VASANT G. HONAVAR

Dr. Vasant Honavar Dorothy Foehr Huck and J. Lloyd Huck Chair in Biomedical Data Sciences and Artificial Intelligence Director, Center for Artificial Intelligence Foundations and Scientific Applications <u>vhonavar@psu.edu</u> College of Information Science and Technology E335 Westgate Building Pennsylvania State University <u>http://faculty.ist.psu.edu/vhonavar</u> 515-451-3507 (cell - preferred), 814-865-3141 (work)

CITIZENSHIP

US Citizen through Naturalization

EDUCATION

University of Wisconsin-Madison, USA	PhD (Advisor: Leonard Uhr, Computer Science)	1990
University of Wisconsin-Madison, USA	M.S. Computer Science	1989
Drexel University	M.S. Electrical Engineering	1984
Bangalore University	B.E. Electronics Engineering	1982

PRIMARY TEACHING AND RESEARCH INTERESTS

Artificial Intelligence, Data Sciences, Machine Learning, Causal Inference, Bioinformatics, Health Informatics, Materials Informatics, Behavioral Informatics, Brain Informatics, Social Informatics, Knowledge Representation and Inference, Collaborative data, and computational infrastructure for collaborative science.

ACADEMIC APPOINTMENTS

2021-	Dorothy Foehr Huck and J. Lloyd Huck Chair in Biomedical Data Sciences and Artificial Intelligence	Penn State Univ.
2021-	Director, Center for Artificial Intelligence Foundations and Scientific Applications	Penn State Univ.
2013-	Professor of Informatics	Penn State Univ.
2013-21	Edward Frymoyer Endowed Professor of IST	Penn State Univ.
2015-	Professor of Computer Science and Engineering	Penn State Univ.
2016-	Professor of Data Sciences	Penn State Univ.
2013-	Director, Artificial Intelligence Research Laboratory	Penn State Univ.
2015-	Associate Director, Institute for Computational and Data Sciences	Penn State Univ.
2016-	Sudha Murty Distinguished Visiting Chair in Neurocomputing & Data Science, School of Automation	Indian Institute of Science
2001-13	Professor of Computer Science	Iowa State Univ.
2002	Visiting Professor, Medical Informatics & Biological Statistics	Univ. of Wisconsin
1996-01	Associate Professor, Computer Science	Iowa State Univ.
1998	Visiting Professor, Computer Science	CMU
1990-96	Assistant Professor, Computer Science	Iowa State Univ.
1986-90	Research Assistant, Computer Science	Univ. Wisconsin
1984-86	Teaching Assistant, Electrical and Computer Engineering	Univ. Wisconsin
1982-84	Teaching Assistant, Electrical and Computer Engineering	Drexel Univ.

LEADERSHIP EXPERIENCE

	Scientific Applications	
2024-	NSF National Synthesis Center for Emergence in the Molecular and Cellular Sciences	Penn State Univ.
2021-22	Program Chair, AAAI Conference on Artificial Intelligence	AAAI
2020-	Cross-Hub Coordination Committee	NSF Big Data Hubs
2020-22	AI and Blockchain Task Force	MDEpinet
2016-21	Co-director, Biomedical Data Sciences PhD Training Program	Penn State Univ.
2016-17	Chair, Data Sciences Faculty Search, College of IST	Penn State Univ.
2016-19	Co-Director, Data Sciences Undergraduate Program, College of IST	Penn State Univ.
2014-	Associate Director, Institute for Computational and Data Sciences	Penn State Univ.
2015-	Director, Center for Big Data Analytics and Discovery Informatics	Penn State Univ.
2015-	Co-director, Informatics, Clinical and Translational Sciences Institute	Penn State Univ.
2014-18	Council Member, Computing Community Consortium	CRA
2015-20	Executive Committee Member	NSF NE Big Data Hub
2010-13	Program Director (IPA), Information and Intelligent Systems Division	NSF
2005-13	Director, Ctr. For Computational Intelligence, Learning, & Discovery	Iowa State Univ.
2006-10	Director of Research, Department of Computer Science	Iowa State Univ.
2009-10	Chair, Promotion and Tenure Committee, Computer Science	Iowa State Univ.
2003-05	Chair, Bioinformatics & Computational Biology Graduate Program	Iowa State Univ.
2003-04	Chair, Research Space Committee, Computer Science	Iowa State Univ.
2002-10	Director of Research, Computer Science	Iowa State Univ.
2001-02	Chair, Graduate Admissions Committee, Computer Science	Iowa State Univ.
2001-03	Associate Chair, Bioinformatics & Comp. Biol. Graduate Program	Iowa State Univ.
1999-01	Chair, Graduate Admissions, Computer Science	Iowa State Univ.
2001	Co-Chair, Strategic Planning, Computer Science	Iowa State Univ.
1999-00	Chair, Graduate Admissions, Bioinformatics & Comp. Biol. Program	Iowa State Univ.
1999-00	Chair, Faculty Search, Computer Science	Iowa State Univ.
1990-13	Founder and Head, Artificial Intelligence Research Laboratory	Iowa State Univ.

INTERDEPARTMENTAL AND INTERDISCIPLINARY PROGRAM PARTICIPATION

Public Health Sciences Graduate Program	Penn State Univ.
Population Research Institute	Penn State Univ.
The Huck Institutes of the Life Sciences	Penn State Univ.
Institute for Computational and Data Sciences	Penn State Univ.
Bioinformatics and Genomics Graduate Program	Penn State Univ.
Operations Research Graduate Program	Penn State Univ.
Neuroscience Graduate Program	Penn State Univ.
Center for Computational Intelligence, Learning, & Discovery	Iowa State Univ.
Bioinformatics & Computational Biology Graduate Program	Iowa State Univ.
Laurence H. Baker Center for Bioinformatics and Biological Statistics	Iowa State Univ.
Computational Molecular Biology Training Group	Iowa State Univ.
Comp. Biol. For Animal Agriculture Training Group	Iowa State Univ.
Human Computer Interaction Graduate Program	Iowa State Univ.
Information Assurance Master's Program	Iowa State Univ.
Information Assurance Center	Iowa State Univ.
Institute for Science and Society	Iowa State Univ.
Neuroscience	Iowa State Univ.
	Population Research Institute The Huck Institutes of the Life Sciences Institute for Computational and Data Sciences Bioinformatics and Genomics Graduate Program Operations Research Graduate Program Neuroscience Graduate Program Center for Computational Intelligence, Learning, & Discovery Bioinformatics & Computational Biology Graduate Program Laurence H. Baker Center for Bioinformatics and Biological Statistics Computational Molecular Biology Training Group Comp. Biol. For Animal Agriculture Training Group Human Computer Interaction Graduate Program Information Assurance Master's Program Information Assurance Center Institute for Science and Society

CAREER HIGHLIGHTS

Pennsylvania State University (2013-Present)

Professor of Information Sciences and Technology:

- Artificial Intelligence Research Laboratory: Led the development of Artificial Intelligence Research Laboratory as a focal point for research in Artificial Intelligence (especially Machine Learning, Causal Inference, Big Data Analytics, Knowledge Representation and applications in Bioinformatics, Health Informatics, and Security Informatics.
- Research and Graduate and Postdoctoral Training: Conceiving and leading research projects in Machine Learning (especially predictive modeling of high-dimensional, longitudinal data, network data), Big Data Analytics, Knowledge Representation (especially secrecy-preserving query answering and preference reasoning) and Causal Inference (especially eliciting causal effects from temporal and relational data), and applications in bioinformatics (especially computational prediction of protein-protein and protein nucleic acid interfaces and complexes, analysis of microbiomes), health informatics (e.g., predictive modeling of health outcomes from clinical, biomedical, environmental, and socio- economic data), and data and computing infrastructure for data-intensive interdisciplinary collaborations, funded in part by grants from the National Science Foundation, the National Institutes of Health, and National Security Agency. Graduated 4 PhD students and currently supervising a research group consisting of 10 PhD Students (7 in Informatics, 2 in Computer Science and Engineering, 1 in Bioinformatics and Genomics).
- Undergraduate and Graduate Programs in Data Sciences: Co-led the establishment of a new innovative inter-college undergraduate degree program in Data Sciences, that combines foundational training in Computing, Informatics, and Statistics (e.g., Statistical Methods, Databases and Data Integration, Programming and Data Structures, Machine Learning, Big Data Algorithms, Programming Models for Big Data, Capstone Project) together with exposure to least one application domain (e.g., Life Sciences, Social Sciences, Business, Health Sciences, Physical Sciences). Developed or co-developed Data Sciences undergraduate courses in Machine Learning, and related topics); Led the design and development of an innovative master's program in Data Sciences (currently in the process of being formalized), co-led the development of an Artificial Intelligence undergraduate program (currently in the process of being formalized).
- Service to the College, University: Institute for Computational and Data Science (ICDS) Associate Director 2014-present, ICDS Faculty Council Member 2020-present, Member of the Data Sciences coordination committee (2020-present), Chair of the Data Sciences Faculty Search Committee (2016-2017), Graduate Recruitment Committee (2016-2017), Faculty Council (2016-2021), Graduate Advisory Committee (2014-2016, 2018-2020), Promotion and Tenure Committee (2016-17), Faculty Evaluation Committee (Research) (2016-2021), Strategic Planning Committee (2015-2016). Led the Data Sciences thrust of the IST strategic plan (2016); Led a major faculty hiring initiative in the Data Sciences (including co-hires in Big Data Life Sciences in coordination with the Huck Institutes of the Life Sciences); Co-led the development of the ICDS strategic initiatives in Data Sciences and Artificial Intelligence, leading to the establishment of several focused research centers, including the Center for Artificial Intelligence Foundations and Scientific Applications; Contributed to the "Driving Digital Innovation" and "Precision Health in Context" thrusts of the University's strategic plan. Mentored junior faculty within and outside the college, e.g., in developing successful NSF CAREER proposals, NIH K proposals, etc.; Served on the College of Medicine Strategic Planning Effort in Artificial Intelligence in Medicine.

Leadership of Interdisciplinary Research Initiatives

Associate Director, PSU Institute for Computational and Data Science (ICDS)

- **Institute Leadership**. Contributed to developing the vision, mission, strategic plan, and priorities of Institute for Computational and Data Sciences, a university-wide institute including in particular, broadening of its focus and mission beyond providing high performance research computing center to fostering research in data and computation intensive discovery across all areas of science and engineering, through strategic faculty co-hires in Data Sciences and AI across the university, initiation of strategic research initiatives, seed grants in support of collaborative research, etc. Served ICDS in a number of capacities including representing ICDS in strategic cohiring of faculty with a number of academic units across the university (e.g., in Data Sciences, Biomedical Sciences, and related areas); representing ICDS in campus-wide initiatives e.g., in Precision Health, Microbiome, Data Sciences; Representing ICDS in strategic planning related activities; Organized seed grant competitions; Mentored junior faculty; Fostered interdisciplinary collaborative research; Developing advanced research computing infrastructure, etc. Led the development of the Scientific Artificial Intelligence initiative, a faculty-led research initiative of the ICDS aimed at elevating Penn State to a position of national leadership in developing and applying cutting edge Artificial Intelligence and machine learning methodologies to advance a number of scientific disciplines, including materials discovery, predictive and causal modeling of health risks and health outcomes, understanding molecular structure, function, and dynamics, among others. Contributed to Penn State's AI and Data Sciences initiatives, including the College of Medicine's strategic investments in AI. Contributed to multiinstitutional partnerships e.g., ERN, Northeast Big Data Hubs aimed at lowering the barriers to collaboration across institutional and disciplinary boundaries.
- Interdisciplinary Center Leadership: Led the development of a Center for Artificial Intelligence Foundations and Scientific Applications that brings together expertise in Artificial Intelligence and Scientific applications across the university to pursue foundational and applied research in AI focused on dramatically accelerating science through advances in scientific knowledge representation, science-informed machine learning, optimal experiment design and execution, and human-AI collaboration. Led an NSF-funded planning of the NSF AI Institute for Materials Discovery. Led the development of the Center for Big Data Analytics and Discovery Informatics cosponsored by the College of Information Sciences and Technology, Institute for Computational and Data Sciences, the Huck Institutes of the Life Sciences, and the Social Science Research Institute that brings together faculty with expertise in computer science, informatics, and statistics with researchers across several scientific domains (Health, Life Sciences, Brain Sciences, Environmental Sciences, Social Sciences, Material Sciences) to pursue foundational research on computational and statistical methods, tools, and data and computing infrastructure and their application to problems of societal importance.
- **Penn State Clinical and Translational Sciences Institute (CTSI)**: Informatics colead of Penn State CTSI (an NIH-funded project with a budget of approximately \$20 million, renewed recently for an additional 5 year period) focused on developing data and computational infrastructure for data access and use policy compliant integration and analyses of clinical, biomedical, socio- demographic, environmental, behavioral, and other types of data for predictive and causal modeling of health outcomes and personalization of interventions, translational applications of artificial intelligence and machine learning in biomedical and health sciences, and education and training of basic

and clinical researchers in biomedical AI. Fostering data and computation-enabled research in the biomedical and health sciences.

- **Virtual Data Collaboratory:** Leading (with Manish Parashar of Rutgers University) the design, implementation, and evaluation of a multi-university distributed cyberinfrastructure for collaborative, data-intensive science; and co-leading (with Helen Berman of Rutgers University), life sciences use case focused on novel methods and distributed workflows for analyses and prediction of protein nucleic acid interactions, interfaces, and complexes (An NSF funded \$4 million, 4-year project).
- Penn State Biomedical Data Sciences (BD2K) Doctoral Training Program: Coled the establishment of a new NIH-funded innovative PhD training program in Biomedical Data Sciences to prepare a diverse cadre of Biomedical Data Scientists with deep expertise in computing, statistics, and informatics and adequate exposure to some area of Biomedical and Health Sciences develop and apply innovative algorithms and statistical methods for predictive and causal modeling of, and effective interventions that impact individual and population health outcomes through integrative analysis of clinical, biomedical, behavioral, socio-economic, environmental, and other types of data.
- **Interdisciplinary Focus Groups**: Initiated interdisciplinary study groups to foster collaborative research at the intersection of Data Sciences and (i) Health Sciences; (ii) Life Sciences; (iii) Brain Sciences; (iv) Material Sciences.
- Service to the Discipline and the Scientific Community
 - Program Chair, AAAI Conference on Artificial Intelligence (2022). As program chair of AAAI-22, the premium national conference on artificial intelligence, oversaw the review process for over 10,000 submissions, and worked with the general chair on all aspects of the technical program.
 - Member, Computing Community Consortium Council (2014-2017), a standing committee of the Computing Research Association, charged by NSF with developing and articulating computing research agendas organized around emerging opportunities or national or societal challenges and priorities, chaired the CCC task force on Convergence of Data and Computing, contributed to task forces on Artificial Intelligence and on Health IT, organized the AAAI/CCC Symposium on "Accelerating Science: A Grand Challenge for AI", led the CCC white paper on "Accelerating Science: Computing Research Agenda", contributed to several CCC white papers and research agenda setting workshops, co-organized the CCC Symposium on Computing Research: Addressing National Priorities and Societal Needs.
 - Electorate Nominating Committee (ENC) member of AAAS Section T. As a member of the electoral nominating committee of the Information, Computing, and Communication Section (Section T) of the American Association for Advancement of Science (AAAS), helped identify candidates for key leadership positions within AAAS Section T.
 - Northeast Big Data Innovation Hub (2015-present) As member of the Executive Committee and Co-PI of the Northeast Big Data Innovation Hub, an NSF-funded consortium of academic, industrial, non- profit organizations aimed at fostering translational data sciences research, education, and workforce development aimed at addressing complex national and regional challenges (e.g., accelerating science, improving health, enabling smart cities and communities), worked with other members of the Hub leadership to develop, articulate, and implement the Hub's vision, strategic priorities, activities. Co-led a successful NSF funded proposal for a 'spoke' on integration and sharing of population health data for data-intensive health research and novel data analytics methods development and evaluation.
 - **Eastern Regional Network** (2016-present) As a member of the steering committee of the

Eastern Regional Network, a consortium of universities in the Eastern region of the United States organized around developing innovative computational and data infrastructure for lowering the barriers to transformative collaborative research that transcends institutional and disciplinary boundaries, conceived, and co-led the planning activities, with support from National Science Foundation.

- NSF AI Institute Planning Effort on AI for Accelerating Materials Discovery, Design, and Synthesis (2020-present). As PI of the NSF-funded project, I led a multi-disciplinary team of investigators across several universities to articulate a shared research agenda for AI and material science, initiate exploratory collaborative research projects, and develop the organizational structure of an interdisciplinary AI institute to make foundational advances in AI motivated by the research challenges in material science.
- National Science Foundation (2010-2013).
 - **BIGDATA: Critical Techniques and Technologies for Advancing Big Data Science and Engineering (2011-2013).** Lead Program Director. Responsible for drafting/revising solicitation, managing program budget, coordination with multiple NSF directorates and NIH institutes, organizing and managing multiple review panels, making funding recommendations, managing awards, communicating with NSF leadership and the broader scientific community, Participating in Interagency Big Data R&D Working Group coordinated by NITRD. In this role, worked closely with multiple NSF directorates as well as other federal agencies (especially NIH) to implement an ambitious, interdisciplinary, big data program.
 - III: Information Integration and Informatics Core Program (2010-2013). Program Director, Responsible for contributing to the solicitation, organizing, and managing multiple review panels for small, medium, large and CAREER proposals, making funding recommendations, managing awards, on a variety of topics related to Data Mining, Machine Learning, Social Networks and Social Media, Information Integration, Bioinformatics, and Semantic Technologies
 - **Expeditions in Computing (2010-2013).** Program Director, co-managing review panels, providing input on funding recommendations, managing 2 expeditions awards (Making Sense at Scale with Algorithms, Machines and People, Understanding Climate Change: A Data Driven Approach), organizing annual reviews and site visits, communicating with NSF leadership and the broader scientific community.
 - SHB: Smart Health and Wellbeing. (2011-2013). Program Director, Responsible for contributing to the solicitation, organizing, and managing multiple review panels, making funding recommendations, managing awards.
 - **SLC: Science of Learning Centers (2011-2013).** CISE representative on the NSF oversight team for the Pittsburgh Science of Learning Center, responsible for project oversight, annual review, and recommendations.
 - **IGERT: Integrative Graduate Education and Research Training (2011-2013).** Program Directors, Responsible for organizing proposal review panels and making funding recommendations on CISE-IIS-relevant proposals.
 - **CRI: Computing Research Infrastructure (2011-2013):** Program Director, Responsible for organizing proposal review panels and making funding recommendations for CISE-IIS-relevant proposals.
 - NRI: National Robotics Initiative (2011-2013). Program Director, Responsible for organizing proposal review panels and making funding recommendations for CISE-IISrelevant proposals.
 - SI²: Software for Sustained Innovation, Program Director, Responsible for co-

organizing panels and making funding recommendations for CISE-relevant proposals.

- Research Planning Workshops: Initiated research planning workshops on
 - Discovery Informatics (organized by Yolanda Gil and Haym Hirsh),
 - Population Health Measurement and Analysis (organized by Bruce Schatz)
 - Finance Informatics (organized by Louiqa Raschid)
 - Knowledge Representation (organized by Natasha Noy and Deborah McGuinness).
- NSF-OFR inter-agency collaborative research initiative in Finance Informatics: Program Director. Responsible for a Dear Colleague Letter and Memorandum of Understanding between NSF and OFR on a joint NSF-OFR initiative focused on algorithms, informatics, knowledge representation, and data analytics needed to advance the current state of the art in financial research and analysis.

• Iowa State University

- **Professor of Computer Science and of Bioinformatics and Computational Biology** (1990-2013)
 - Research: Foundational contributions in Machine learning, Data Mining, Knowledge Representation and Semantic Web and interdisciplinary contributions in Bioinformatics and Computational Biology: Scalable approaches to learning predictive models from very large, distributed, data; Methods for learning predictive models from richly structured data (including tabular, sequence, network, relational, linked open, multi-modal, time series data); Learning regular and stochastic context free grammars; Eliciting causal information from multiple sources of observational and experimental data; Selective sharing of knowledge across disparate knowledge bases, including novel approaches to secrecy-preserving query answering; Representing and reasoning about preferences; Composing complex software services from components; and applications in bioinformatics and computational molecular and systems biology, including methods and software for characterization, analysis, and prediction of sequence and structural correlates of protein- protein, and protein-RNA interfaces interactions, comparative analyses biological and of networks (http://ailab.ist.psu.edu/software.html).
 - **Teaching and Curriculum Development:** Established, and over the years, refined and broadened graduate and undergraduate curricula, integration of research into undergraduate education in Artificial Intelligence and Machine Learning.
 - Artificial Intelligence Laboratory: Established and led Artificial Intelligence Research Laboratory as a focal point for AI research at Iowa State University. The laboratory secured over \$20 million in research funding from NSF, NIH, USDA, and DOD trained 30 PhD students (10 employed as tenure-track or tenured faculty in academia, 10 employed in academic research, and 10 employed in industrial research and development), 25 MS graduates (24 employed in industry, one in academic research).
 - Center for Computational Intelligence, Learning and Discovery (2005-2013). Established and led an interdisciplinary research center focused on foundational research in Computer Science (AI, Machine Learning, Informatics, Theoretical Computer Science, Algorithms, Systems), Statistics, and application areas such as Life Sciences, Agriculture, Engineering.
 - Interdepartmental PhD Program in Bioinformatics and Computational Biology: Coled the establishment of the interdepartmental graduate program in Bioinformatics and Computational Biology, with support from an NSF Integrative Graduate Education and Research Training (IGERT) award in 2000, renewed for a second 5-year period in 2005, and

served as associate chair (2001-2003) and chair (2003-2005) of the of the program during its formative years. Lead a major curriculum development effort focused on required core courses for the graduate program in Bioinformatics and Computational Biology, culminating in the creation of a Bioinformatics graduate core curriculum comprising of 4 core courses covering Genomics to Systems Biology. By 2005, the program was one of the top graduate programs in Bioinformatics among institutions without a medical school.

- Undergraduate Program in Bioinformatics and Computational Biology: Co-led the development of an undergraduate curriculum and the establishment of interdepartmental undergraduate degree program in Bioinformatics and Computational Biology in 2007.
- Service to the Department, College, and University: Served the Department of Computer Science in several important roles including Director of Research (2006-2011) responsible for research infrastructure and fostering research collaborations with other disciplines; Committees focused on Strategic Planning, Faculty hiring, Promotion and tenure, Graduate Admissions, Graduate Curriculum, among others; university research computing advisory committee, among others.
- Service to the Discipline and the Scientific Community: Service on NIH Study Sections, including Charter member of NIH study section on Biological Data Management and Analysis (2004-2007), NSF Proposal Review panels, Editorial boards of several journals, Organization of several scientific conferences and workshops.

BIOGRAPHICAL SUMMARY

Dr. Vasant Honavar received his Ph.D. in Computer Science and Cognitive Science in 1990 from the University of Wisconsin Madison, specializing in Artificial Intelligence. In September 2013, Honavar joined the faculty of Penn State University where he currently holds the Dorothy Foehr Huck and J. Lloyd Huck Chair in Biomedical Data Sciences and Artificial Intelligence after having held the Edward Frymover endowed Chair in Information Sciences and Technology during 2013-2021. He is the founding Director of the Center for Artificial Intelligence Foundations and Scientific Applications, Associate Director of the Institute for Computational and Data Sciences, Co-Director of the NIH-funded Biomedical Data Sciences PhD program, and Informatics lead (research) for the NIH- funded Clinical and Translational Sciences Institute, Co-PI of the Northeast Big Data Hub, PI of the NSF planning grant for an Institute for AIenabled Materials Design, Discovery, and Synthesis, and Co-PI of the NSF Eastern Regional Network Midscale Infrastructure planning project. Honavar serves on the faculty of the Computer Science, Bioinformatics and Genomics, Neuroscience, and the Operations Research Graduate Programs and the Data Sciences undergraduate program at Pennsylvania State University. In 2016, Honavar was appointed as the Sudha Murty Distinguished Visiting Chair of Neurocomputing and Data Science at the Indian Institute of Science. Honavar served as a member of the Computing Community Consortium Council (CCC) where he chaired the Convergence of Data and Computing Task Force (2015-2017) and served on Artificial Intelligence and Health IT task forces, and as a member of the FDA's MDEpinet Blockchain and AI Taskforce (2020-21). Dr. Honavar served on the Executive Committee of the NSF Northeast Big Data Innovation Hub (2016-2020) and currently serves on the Cross-Hub Coordination Committee. During 2015-2018 he served as a member of the Electorate Nominating Committee of the Section on Information, Computing, & Communication of the American Association for the Advancement of Science (AAAS). Honavar served as a program co-chair of the 2022 AAAI Conference on Artificial Intelligence. In addition to research, graduate student supervision and teaching, he is responsible for developing new research and educational initiatives in Data Sciences and contributing to research initiatives in Biomedical and Health Sciences.

From 1990 to 2013, Honavar served on the faculty of Computer Science and of Bioinformatics and Computational Biology at Iowa State University (ISU). At ISU, he directed the Artificial Intelligence

Research Laboratory (which he founded in 1990) and the Center for Computational Intelligence, Learning & Discovery (which he founded in 2005) and served as the associate chair (2001-2003) and chair (2003-2005) of the ISU Bioinformatics and Computational Biology Graduate Program, which he helped establish in 1999 with support from an Integrative Graduate Education and Research Training (IGERT) award. During 2010-2013, Honavar served as a program director in the Information and Intelligent Systems Division of the Computer and Information Sciences and Engineering directorate of the National Science Foundation (NSF) during 2010-2013 while maintaining his research program at ISU. He led the Big Data Science and Engineering Program, established the NSF-OFR collaboration in Computational and Information Processing Approaches to and Infrastructure in support of, Financial Research and Analysis and Management, contributed to Smart and Connected Health, Information Integration and Informatics, Expeditions in Computing, Science of Learning Centers, Integrative Graduate Education and Research Training, Computing Research Infrastructure Programs.

Honavar's current research and teaching interests include Artificial Intelligence, Machine Learning, Bioinformatics, Causal Inference, Data Sciences, Information Integration, Knowledge Representation and Inference, Bioinformatics, Biomedical and Health Informatics, Materials Informatics, Social Informatics, and Security Informatics. Honavar has led research projects funded by NSF, NIH, and USDA that have resulted in foundational research contributions (documented in over 300 peer-reviewed publications, that have been cited over 19000 times, or over 500 citations on average per year during 1990-2024, hindex=64) in: scalable approaches to learning predictive models from very large, richly structured data (including tabular, sequence, network, relational, time series data); Eliciting causal information from multiple sources of observational and experimental data, Selective sharing of knowledge across disparate knowledge bases, including novel approaches to secrecy- preserving query answering; Representing and reasoning about preferences; Composing complex software services from components; and applications in bioinformatics and computational molecular and systems biology (including characterization, analysis, and prediction of sequence and structural correlates of protein- protein, and protein-RNA interfaces and interactions, comparative analysis of biological networks (network alignment)). This research has resulted in a broad range of software and tools (See http://ailab.ist.psu.edu/software.html). Honavar's current research is focused on the theoretical foundations and algorithms for eliciting causal effects from relational and temporal data; for machine learning algorithms for predictive modeling from large, heterogeneous, high dimensional, richly structured, longitudinal data, with applications in biomedical, health, behavioral and cognitive sciences, and related areas: algorithms for modeling and comparative analyses of brain networks structure and dynamics from fMRI, diffusion tensor imaging and other data; development of a distributed computing and data infrastructure for collaborative data intensive research, analyses and prediction of protein- nucleic acids interactions, interfaces and complexes, analysis and modeling of microbiomes. Honavar has served as a principal or co-principal investigator on grants totaling over \$80 million during 1990-2021 from the National Science Foundation, the National Institutes of Health, the US Department of Agriculture, the US Department of Defense, and the National Security Agency. He has extensive curriculum development and teaching experience in Artificial Intelligence, Machine Learning, and Bioinformatics. He also has substantial industrial consulting experience in Artificial Intelligence, Machine Learning, Data Sciences, Bioinformatics, and related topics.

Honavar has served on, or currently serves on the editorial boards of several journals including IEEE/ACM Transactions on Computational Biology and Bioinformatics, Springer Open Journal of Big Data, Journal of Computational Systems Biology, Cognitive Systems Research, Machine Learning, the Journal of Bioinformatics and Biology Insights, the International Journal of Semantic Web and Information Systems, the International Journal of Computational Biology and Drug Design, the International Journal of Computer and Information Security, and the International Journal of Data Mining and Bioinformatics among others.

Honavar served as a Program Chair of the 36th Conference on Artificial Intelligence (AAAI-22), the

premier research conference of the Association for the Advancement of Artificial Intelligence. He served as a general co-chair of the 2014 IEEE International Conference on Big Data in 2014 and the program co-chair of 2014 IEEE Conference on Bio and Medical Informatics. Honavar has served as a member of the Board of Directors for ACM Special Interest Group on Bioinformatics, scientific program committees of major research conferences in artificial intelligence, data mining, and bioinformatics including the member of the Board of Directors for ACM Special Interest Group on Bioinformatics, scientific program committees of major research conferences in artificial intelligence, data mining, and bioinformatics including the Conference on Artificial Intelligence (AAAI), International Conference on Machine Learning (ICML), ACM SIGKDD Conference on Knowledge Discovery and Data Mining (KDD), SIAM Conference on Data Mining (SDM), IEEE Conference on Data Mining (ICDM), Intelligent Systems in Molecular Biology (ISMB), ACM Conference on Bioinformatics and Computational Biology (ACM-BCB), among others. Honavar has served on multiple NIH Study Sections and including a charter member of the National Institutes of Health study section on Biological Data Management and Analysis (2002-2007). Honavar is a senior member of the Association for Computing Machinery (ACM), the Institute of Electrical and Electronic Engineers (IEEE) and the Association for Advancement of Artificial Intelligence (AAAI); and a member of International Society for Computational Biology (ISCB) Society for Industrial and Applied Mathematics, and the American Association for the Advancement of Science.

Honavar has received many awards and honors during his career including Dorothy Foehr Huck and J. Lloyd Huck Chair in Biomedical Data Sciences and Artificial Intelligence at the Pennsylvania State University in 2021, Fellow of the American Association for Advancement of Science (AAAS) in 2018, the National Science Foundation Director's Award for Superior Accomplishment in 2013 for his leadership of the NSF Big Data Program, the National Science Foundation Director's Award for Collaborative Integration in 2011, the Pennsylvania State University College of Information Sciences and Technology Senior Faculty Excellence in Research Award in 2016, the Sudha Murty Distinguished Visiting Chair in Neurocomputing and Data Science at the Indian Institute of Science in 2016, the Edward Frymoyer Endowed Professorship in Information Sciences and Technology at Pennsylvania State University College of Liberal Arts and Sciences Award for Career Excellence in Research 2008, and the Iowa State University Margaret Ellen White Graduate Faculty Award in 2011. However, his proudest accomplishments are the 39 PhD students, 32 MS Students, and many undergraduate researchers that he has worked with and mentored during his career.

HONORS AND AWARDS

	HOHORS AND AWARDS	
2021-	Dorothy Foehr Huck and J. Lloyd Huck Chair in Biomedical Data Sciences and Artificial Intelligence, Penn State Univ.	
2018	American Association of Advancement of Science (AAAS) Fellow	
2018	ACM Distinguished Member Award	
2016-	Sudha Murty Distinguished Visiting Chair in Neurocomputing and Data Science, IISc	
2016	125 People of Impact, Dept. of Electrical and Computer Engg., Univ. Wisconsin	
2016	Senior Faculty Research Excellence Award, College of IST, Penn State Univ.	
2014-17	Council Computing Community Consortium, Computing Research Assoc.	
2014	Senior Member, Association for the Advancement of Artificial Intelligence	
2013-	Edward Frymoyer Endowed Professorship in Information Sciences and Technology	
2013	National Science Foundation Director's Award for Superior Accomplishment	
2013	Best Student Paper Award (PhD student Harris Lin), IEEE Big Data Congress, 2013	
2012	National Science Foundation Director's Award for Collaborative Integration	
2011	Margaret Ellen White Graduate Faculty Award, Iowa State University	
2011	Best poster award, ACM Conference on Bioinformatics and Computational Biology	
2011	Elected Fellow, International Society for Intelligent Biological Medicine	
2008	Liberal Arts and Sciences Award for Excellence in Research, Iowa State University	

2007	Regents Award for Faculty Excellence, Board of Regents, Iowa	
2006	Best Paper Award, Asian Semantic Web Conference	
2006	Best Paper Award, IEEE ICTAI 2006	
2006	Senior Member, Association for Computing Machinery	
2001	Senior Member, IEEE	
1994-99	Research Initiation Award, National Science Foundation	
1994	Who's who in Science and Engineering	
1992	Elected Member, Sigma Xi	
1990-	Associate, Behavior and Brain Sciences	
1990	Elected Member, New York Academy of Sciences	
1990	Fellow, Workshop on Human and Machine Cognition	
1989	Fellowship, Summer Institute in Parallel Computing, Argonne National Laboratory	
1989	Student Fellowship, International Joint Conference on Artificial Intelligence (IJCAI)	
1989	Fellowship, McDonnell Summer Institute in Cognitive Neuroscience, Dartmouth	
1988	Fellowship, Connectionist Models Summer School, Carnegie Mellon University	
1982	Gold medal for academic excellence, Bangalore University, India	
1975-82	National Merit Scholar, India	

EDITORIAL BOARDS

erJournal of Computational Systems BiologyerJournal of Cognitive Systems ResearcherSpringer Open Journal of Big Data	
er Springer Open Journal of Big Data	
IEEE/ACM Transactions on Bioinformatics and Comp. Biol.	
er Journal of Bioinformatics and Biology Insights	
er Intl. J. Computational Biology and Drug Design	
er Intl. J. Functional Informatics & Personalized Medicine	
er Applied Intelligence Journal	
er Intl. J. Semantic Web and Information Systems	
Springer Book Series: Advanced Info. & Knowledge Proc.	
Machine Learning Journal	
Cognitive Systems Research	
er Intl. J. Data Mining and Bioinformatics	
er Intl. J. Information and Computer Security	
Machine Learning Journal	

STUDY SECTION AND REVIEW PANEL MEMBERSHIP

2024	Clinical Informatics and Digital Health Panel	NIH
2023	Proposal Review Panels	NSF
2022	Proposal Review Panels	NSF
2021	Special Emphasis Panel	NIH
2021	Canada Research Chairs Review Panel	Canada Res. Chairs
2020	Proposal Review Panels	NSF
2020	Special Emphasis Panel	NIH
2019	Proposal Review Panels	NSF
2018	Proposal Review Panels	NSF
2017	Proposal Review Panels	NSF
2016	Proposal Review Panels	NSF
2016	SBE Proposal Review Panel	NSF

2016	Special Emphasis Panel, BD2K T32	NIH
2016	Special Emphasis Panel, Precision Health Cohorts	NIH
2016	NCATS Special Emphasis Panel	NIH
2016	NIAIDS Special Emphasis Panel	NIH
2016	Canada Research Chairs Review Panel	Canada Res. Chairs
2015	NCATS Special Emphasis Panel	NIH
2015	NCI Special Emphasis Panel	NIH
2015	SBE Proposal Review Panel	NIH
2015	NIAIDS Special Emphasis Panel	NIH
2015	Special Emphasis Panel, BD2K T32	NIH
2014	CISE Proposal Review Panel	NSF
2014	NAGMS Council (ad hoc member)	NIH
2013	CISE Proposal Review Panel	NSF
2013	Proposal Review Panel	DOE
2010	Special Emphasis Study Section, Natl. Ctr. For Res. Resources	NIH
2010	National Centers for Biomedical Computing Review Panel	NIH
2010	Study Section, Biological Data Management and Analysis	NIH
2010	CISE Review Panels	NSF
2009	Bioinformatics Resource Centers for Infectious Diseases	NIH
2009	Genomics, Bioinformatics and Systems Biology Review Panel	European Res. Council
2009	Review Panel	Canada Res. Chairs
2009	CISE Review Panel	NSF
2008	CISE Review Panel	NSF
2008	Study Section Chair, Data Ontologies, Sharing Data & Tools	NIH
2004-07	Biological Data Management & Analysis	NIH
2006	CISE Review Panel	NSF
2005	CISE Review Panel	NSF
2004	Special Study Section, NIH Roadmap Initiative	NIH
2004	Special Study Section, Data Sharing Initiative	NIH
2001-04	Special Study Section, Bioinformatics	NIH
2003	CISE Intelligent Information Systems Review Panel	NSF
2003	CISE CAREER Review Panel	NSF
2003	SBIR Review Panel	NSF
2003	SBIR Review Panel	NSF
1999	IGERT Review Panel	NSF
2002	CISE Review Panel	NSF
1994	CISE Review Panel	NSF

PROFESSIONAL AFFILIATIONS

2014-	Senior Member, AAAI, Association for Advancement of Artificial Intelligence)	
1986-2014	Member, AAAI (Association for Advancement of Artificial Intelligence)	
2007-	Senior Member, ACM (Association for Computing Machinery)	
2005-	Senior Member, IEEE (Institute of Electrical and Electronic Engineers)	
1990-	Member, Institution of Electrical and Electronic Engineers (IEEE)	
1990-2005	Member, IEEE Computer Society	
1990-2007	0-2007 Member, Association of Computing Machinery (ACM)	
1992-	1992- Member, American Association for Advancement of Science	
1998-	8- Member, Cognitive Science Society	

RESEARCH STATEMENT

Current Research Interests

- 1. **Artificial Intelligence:** Logical, probabilistic, causal, and decision-theoretic knowledge representation and inference, Neural architectures for knowledge representation and inference.
- 2. **Machine Learning and Data Science:** Statistical, information theoretic, linguistic and structural, relational, neural network, decision theoretic approaches to machine learning. Federated machine learning. Continual learning. Physics-based machine learning. Multi-modal and multi-fidelity learning; Causal learning. Learning predictive models from tabular, relational, text, image, genomic, time series, longitudinal, spatio-temporal and network data; Bias and fairness in machine learning; Explainable and interpretable machine learning.
- 3. **Causal Models:** Estimating causal effects from observational data including tabular, relational, and temporal data; Learning causal models from data; Generalizability of causal effects across settings; Causal explanations.
- 4. **AI for Science:** Computational models of scientific discovery; Discovery informatics infrastructure to integrate data, hypothesis, and knowledge-based inference, predictive modeling, experimentation, simulation, and hypothesis testing to provide an orderly formal framework and exploratory apparatus for science; Applications in life sciences, health sciences, materials sciences.
- 5. Knowledge Representation and Inference: Probabilistic, logical, grammatical, structural, and neural knowledge representation and inference; federated data and knowledge bases, federated query answering, reasoning, knowledge sharing; federated services service composition, substitution, and adaptation; epistemic description logics; secrecy-preserving query answering, representing and reasoning about single and multi-stakeholder qualitative preferences; representing and reasoning about causality.
- 6. **Information Integration:** Probabilistic, network based, relational, logical, knowledge-based, and representation learning approaches to information integration.
- 7. **Bioinformatics and Computational Molecular and Systems Biology:** Computational analyses and prediction of macromolecular sequence-structure-function-interaction-expression relationships, identification of sequence and structural correlates of protein-protein, protein-RNA, and protein- DNA interactions, protein sub-cellular localization, automated protein structure and function annotation, modeling and inference of genetic regulatory networks from gene expression (micro- array, proteomics) data, modeling and inference of signal transduction and metabolic pathways, comparative analysis of biological networks (network alignment), integrative analysis of molecular interaction networks and macro-molecular interfaces.
- 8. **Computational Materials Design, Discovery, and Synthesis.** Foundation models for materials discovery; optimizing material synthesis using machine learning; learning of universal interatomic potentials and thermodynamic equations; inverse materials design; materials property prediction; multi-modal materials characterization; closed-loop integration of data, knowledge, simulations, experiments, and human-AI interactions for materials design, discovery, and synthesis.
- Predictive and Causal Modeling of Health Risks and Health Outcomes. Machine learning methods for predictive modeling of health risks from longitudinal, multi-modal, clinical (electronic health records), socio-demographic and environmental data; Estimating causal effects from clinical data. Biomedical image analysis. Biomedical text analysis.
- 10. **Other Topics of Interest:** Applied machine learning and applied causal inference. Biological Computation, Sensory systems and behavior evolution, Language evolution, Mimetic evolution; Computational Semiotics Origins and use of signs, emergence of semantics; Computational

organization theory; Computational Neuroscience; Computational models of creativity, Computational models of discovery.

My research spans both foundations of AI and applications of AI and is motivated by questions of scientific or societal importance, such as the following:

- How can AI systems augment human intellect to dramatically accelerate science?
- How can we efficiently build robust and explainable predictive models from data?
- How can we elicit causal relations from multiple disparate observational and experimental studies?
- How can we ensure that AI systems are fair, explainable, and accountable?
- How can we build predictive models from federated data?
- How can we build predictive models from multi-modal (multi-view) data?
- What are the information requirements of learning in specific settings?
- How can we learn language syntax (grammars) and semantics?
- How can we build predictive models from high-dimensional longitudinal data?
- How can we construct computational abstractions of scientific artifacts and scientific domains?
- How can we efficiently represent and reason about preferences?
- How can we query and reason with federated data and knowledge bases?
- How can we assemble, adapt, and execute complex services from component services?
- How can we answer queries against knowledge bases without revealing secrets?
- How can we build systems for data access and use policy compliant data integration and analysis?
- How can we learn to predict health risks and outcomes multi-modal longitudinal health data?
- How can we predict macromolecular interactions, interfaces, and complexes?
- How can we construct, compare, and analyze models of molecular networks?
- How can we model, construct, compare, and analyze brain networks from data?
- How can we build systems that learn continually from observations and interactions?
- How can we reduce the energy footprint of AI and machine learning?
- How can we build robust intelligent agents that incorporate multiple facets of intelligence?

My research contributions have spanned Computer Science (especially on the topics of Machine Learning and Data Mining, Knowledge Representation and Inference, Causal Inference) and in Bioinformatics and Computational Biology (especially on the topic of analysis and prediction of biomolecular (proteinprotein, protein-DNA, and protein-RNA) interfaces and comparative analysis of biomolecular interaction networks). Some of my most recent work has focused on (i) Scalable algorithms for building predictive models from large, distributed, semantically disparate data (big data), including more recently, linked open data (ii) Algorithms for constructing predictive models from sequence, image, text, multi-relational, graph-structured data; (iii) New approaches to selective sharing of knowledge across autonomous knowledge bases (including knowledge base federation, secrecy-preserving query answering); (iv) Theoretically sound yet practically useful approaches to functional and non-functional specification driven composition of complex services from components; (v) Expressive languages for representing, and model checking approaches to reasoning with, gualitative preferences; (vi) Algorithms for eliciting causal effects from disparate sources of observational and experimental data; (vii) Scalable algorithms and software for comparative analyses of large bio- molecular networks and (viii) Machine learning approaches to analysis and prediction of macromolecular interactions and interfaces with applications in the analysis and prediction of protein-protein, protein-DNA, and protein-RNA interactions and interfaces, B-cell and T-cell epitopes.

Over the next 5-10 years, I plan to focus my research on (1) Computational abstractions scientific artifacts (e.g., data, knowledge, hypotheses), and universes of scientific discourse (e.g., biology), and scientific processes (e.g., hypothesis generation, predictive modeling, experimentation, simulation, and hypothesis testing), cognitive tools that augment and extend human intellect; and human- machine cyberinfrastructure (including organizational structures and processes) to accelerate science; (2) Design and analysis of algorithms for predictive modeling from very large, high dimensional, richly structured, multi-modal, longitudinal data; (3) Development of theoretically sound and practically useful characterizations and algorithms for continual learning; f(3) Elucidation of causal relationships from disparate experimental and observational studies and from relational, temporal, and temporal-relational data; (4) Design and analyses of accountable, explainable, and fair AI systems; (5) Analysis and prediction of macromolecular interactions, elucidation of complex biological pathways e.g., those involved in immune response, development, and disease; (7) Predictive and causal modeling of individual and population health outcomes from behavioral, biomedical, clinical, environmental, socio- demographic data; (8) Predictive and causal modeling of behavioral and cognitive systems in naturalistic settings; (9) Predictive modeling of material properties from composition and adaptive design of materials; (10) Predictive and causal modeling of behavior and cognition in naturalistic settings.

RESEARCH, TRAINING, AND INFRASTRUCTURE GRANTS Current Research, Training, and Infrastructure Grants

- 1. Honavar, V. (PI). Learning Predictive Models from High-Dimensional, Irregularly and Sparsely Sampled Longitudinal Data. National Science Foundation, \$600,000, 2022-2025.
- Honavar, V. (PI), "Collaborative Research: RI: III: SHF: Small: Multi-Stakeholder Decision Making: Qualitative Preference Languages, Interactive Reasoning, and Explanation". National Science Foundation. \$299,992. 2022-2025.
- 3. Honavar V. (Co-PI). National Synthesis Center for Emergence in Molecular and Cellular Sciences. \$20,000,000. National Science Foundation. 2024-2029.
- 4. Penn State Clinical and Translational Science Institute, Vasant Honavar (Co-I), National Institutes of Health, \$22,113,244. 2021-2026.
- 5. Honavar, V. (Co-I), AI-based Mapping of Complex Cannabis Extracts in Pain Pathways National Institutes of Health, \$3,500,000, 2023-2028.
- Honavar, V. (Co-PI). Collaborative Research: RESEARCH-PGR: Genetic and environmentally induced functional variation in the rice RNA structurome. National Science Foundation. \$1,800,000, 2021-2025.
- 7. Honavar, V. (Co-PI). Collaborative Research: FW-HTF-RL: Future of Digital Facility Management (Future of DFM). National Science Foundation. \$775,438, \$2024-2027
- 8. Honavar, V. (Co-PI). BD Hubs: NORTHEAST: The Northeast Big Data Innovation Hub. National Science Foundation, \$4,000,000. 2019-2023. Administered by Columbia University.
- 9. Honavar, V. (Mentor). Using machine learning to analyze integrated clinical and geo-social data to inform the design of a decision support system to reduce the risk of stimulant therapy. National Institutes of Health, \$960,658. 2024-2029.

Pending Grant Proposals

- Honavar, V. (Co-I). Alzheimer's Disease and Untreated Insomnia (ADIUS): Leveraging Real-World Data to Address Geographic Access Disparities. \$1,655,162. National Institutes of Health. 2025-2030.
- 2. Honavar, V. (Co-PI). Genetic Epidemiology of Aromatase Inhibitor Musculoskeletal Syndrome (AIMSS) in Breast Cancer Patients. National Institutes of Health. \$1,488,738. 2025-2030. Under

revision.

- Honavar, V. (Co-I). Leveraging Electronic Health Records, Brain Health, and Social Determinants of Health to Predict Dementia and Late Seizures After Stroke: A Machine Learning Approach. \$3,152,313. National Institutes of Health. 2025-2030. Under revision.
- Honavar. V. (Co-PI). Research Infrastructure: CIRC: New: A Community Research Infrastructure for Federated Analytics of Integrated Network Data with Threat Intelligence, National Science Foundation, \$1,993,525
- 5. Honavar. V (Co-I). Investigating Factors and Processes Affecting Stroke Readmission Using System Dynamics and Machine Learning. National Institutes of Health. \$4,088,935 Under revision.
- 6. Honavar, V. (Co-I) Leveraging Electronic Health Records, Brain Health, and Social Determinants of Health to Predict Dementia and Late Seizures After Stroke: A Machine Learning Approach. National Institutes of Health. \$3,152,213. 2025-2030.

Past Research and Training Grants

- 1. Honavar, V. (PI). Interpreting Black-Box Predictive Models Through Causal Attribution. National Science Foundation. \$200,000. 2020-2023.
- 2. Honavar, V. (PI). AI Institute: Planning: Institute for AI-Enabled Materials Discovery, Design, and Synthesis. National Science Foundation. \$500,000. 2020-2024.
- 3. Honavar, V. (Co-PI). CC* CRIA: The Eastern Regional Network. National Science Foundation. \$202,618. 2020-2023. Administered by Rutgers.
- Honavar, V. (Co-PI). Research Infrastructure: CCRI: Planning Grant: A Community Research Infrastructure for AI-Enabled Integrated Malware and Network Data Analytics, National Science Foundation, \$100,000. 2022-23.
- 5. Honavar, V. (Co-PI). Exploring Graph Neural Networks for Attributed Multi-Layer Criminal Network Analysis, Center for Criminal Network Analysis, George Mason University, Subaward from Department of Homeland Security, \$340,000, 2022-2024.
- Honavar, V. (PI), "CIF21 DIBBs: EI: Virtual Data Collaboratory: A Regional Cyberinfrastructure for Collaborative Data Intensive Science," National Science Foundation, Collaborative Project with Rutgers University, Total budget: \$4,000,000. Penn State Budget: \$1,482,149. 2017 -2022.
- Honavar, V. (PI), "BD Spokes: SPOKE: NORTHEAST: Collaborative Research: Integration of environmental factors and causal reasoning approaches for large-scale observational health research," National Science Foundation, Collaborative Project with Harvard, Columbia, and CMU. Total budget: \$1,000,000. Penn State Budget: \$95,367. 2017 – 2021.
- 8. Honavar, V. (Co-PI). Graph Optimization via Deep Learning. Samsung Advanced Institute of Technology. \$146,661. 2020-2021.
- 9. Honavar, V. (PI). Predictive Maintenance using machine learning. Volvo, Inc. \$100,000, 2021-2022.
- 10. Honavar, V. (Co-PI). Scalable Near-Real-Time Identification and Characterization of Malware Behaviors from Darknet Data. William J. Hughes Technical Center. \$499,687. 2019-2021.
- 11. Honavar, V., Ritchie, M. D., Li, R. (PIs), "Biomedical Big Data to Knowledge (B2D2K) Training Program," National Institutes of Health, \$1,604,971.00. 2016 2021.
- 12. Penn State Clinical and Translational Science Institute, Vasant Honavar (Informatics lead), National Institutes of Health, \$20,000,000. 2016-2021.
- 13. Honavar, V. (PI), "Towards Computational Infrastructure for Analysis of Sensitive Data," National Science Foundation, \$231,578. 2015 2018
- 14. Honavar, V. (PI), "SHF: Large: Collaborative Research: Inferring Software Specifications from Open-Source Repositories by Leveraging Data and Collective Community Expertise," National Science

Foundation, Collaborative Project with a budget of \$2.5 million, Penn State Budget: \$319,511.00. 2015 – 2020.

- 15. Honavar, V. (PI), "Automating Artificial Intelligence: Empowering Analysts with Intelligent, Autonomous Software Agents," NGIA (Subaward from Concurrent Technologies Corporation), Federal Agencies. \$67,279. 2017.
- 16. New Techniques Towards Active Cyberdefense, National Security Agency, Vasant Honavar (Co-PI), \$275,143.00. 2015 2016.
- 17. Identifying porcine genes and gene networks involved in effective response to PRRS virus using functional genomics and systems biology, Joan Lunney (PI), Vasant Honavar (Co-PI), Zhihua Jiang (Co-PI), Roman Pogranichniy (Co-PI), Juan Pedro Steibel (Co-PI), Chris Tuggle (Co-PI), United States Department of Agriculture, 2010-2014, \$750,000.
- 18. Honavar, V. (Mentor), Coffman, D. L., Li, R., Fellowship, "Novel Methods to Identify Momentary Risk States for Stress and Physical Inactivity," National Institutes of Health, \$500,000.00. 2014- 2017).
- 19. Collaborative Research: Learning Classifiers from Autonomous, Semantically Heterogeneous Distributed Data Sources, National Science Foundation, Vasant Honavar (PI) \$527,000 (including supplements). 2007-2013.
- 20. Intergovernmental Personnel Act (IPA) Appointment, Program Director, Information Integration and Informatics Program, Information and Intelligent Systems Division, Computer and Information Science and Engineering Directorate, National Science Foundation, \$701,972. 2010-2013
- 21. IGERT: Computational Molecular Biology Training Program. Vasant Honavar (Co-PI) with Dan Voytas (PI), Drena Dobbs (Co-PIs). National Science Foundation, 2005-2012. \$2,968,976.
- 22. High-Accuracy Protein Models Derived from Lower Resolution Data. National Institutes of Health (2007-2010), Vasant Honavar (Co-PI), with Andrzej Kloczkowski (PI), Robert Jernigan, Mark Gordon, Zhijun Wu, Iowa State University and Janusz Bujnicki, Krzysztof Ginalski and Andrzej Kolinski, Warsaw University (Co-PIs), \$744,725.
- Interactive and Verifiable Composition of Web Services to Satisfy End User Goals. National Science Foundation, Vasant Honavar (Co-PI), with Samik Basu (PI) and Robyn Lutz (Co-PI). (2007-2011), \$350,002.
- 24. Machine Learning Algorithms and Software for Collaborative Medical Decision Support. Grow Iowa Values Fund, and Collaborative Health Solutions, LLC 2010-2012, \$238,586.
- 25. Developing Predictive Models for Identifying Pigs with Superior Immune Response and Improved Food Safety, Chris Tuggle (PI), Bearson, S., Honavar, V., Nettleton, D. Wannemuehler, M., Lunney, J. and Nettleton, D. (Co-Pis). United States Department of Agriculture (2009-2012), \$1,000,000.
- 26. NIH-NSF BBSI Summer Institute in Bioinformatics and Computational Biology Iowa State University. National Science Foundation, Vasant Honavar (Co-PI) with Volker Brendel (PI), Robert Jernigan, Karin Dorman, and Julie Dickerson (Co-Pis) (2006–2010). \$499,000.
- 27. Development of bioinformatics resources to transfer biological information across species. *United States Department of Agriculture.* Vasant Honavar (Co-PI), James Reecy (PI), Anne Kwitek (Co-PI). (2008-2010). \$1,000,000
- 28. DDAS-TMRP: Auto-Steered Information-Decision Processes for Electric Power Systems Asset Management. *National Science Foundation,* Vasant Honavar (Co-PI) with James McCalley (PI), Sarah Ryan (Co-PI), William Meeker (Co-PI), and Daji Qiao (Co-PI). (2006-2011) \$700,000.
- 29. Discovering Protein Sequence-Structure-Function Relationships. National Institutes of Health Vasant Honavar (PI), Robert Jernigan and Drena Dobbs (Co-Pis), (2003-2008). \$1,022,000.
- 30. IIS: Exploratory Investigation of Modular Ontologies. *National Science Foundation*, Vasant Honavar (PI), Giora Slutzki and Doina Caragea (Co-Pis), (2006-2008). \$112,000.

- 31. Integration of Functional Genomics and Quantitative Genetics to Improve Feed Efficiency in Pigs. United States Department of Agriculture (2005-2008), Vasant Honavar (Co-PI) with Jack Dekkers (PI), Chris Tuggle (Co-PI), Dan Nettleton (Co-PI), Lloyd Anderson (Co-PI), Rondhane Rekaya (Co- PI), Richard Barb (Co-PI), and Gary Hausman (Co-PI), \$876,000.
- 32. Computational Support Staff for Expanding Animal Functional Genomics Capabilities. Vasant Honavar (PI), Chris Tuggle, Jim Reecy, Diane Spurlock, Jack Dekkers, Susan Lamont, Chad Stahl (Co-Pis), \$50,000. (2007-2009).
- 33. Center for Computational Intelligence, Learning, and Discovery. Vasant Honavar (PI). Vice Provost for Research, Iowa State University (2004-2009) \$477,500
- 34. ITR: Algorithms and Software for Knowledge Acquisition from Heterogeneous Distributed Data. *National Science Foundation*, Vasant Honavar (PI) Drena Dobbs (Co-PI), (2002-2007). \$223,500.
- 35. Algorithms and Software for Collaborative Ontology Development. Center for Integrated Animal Genomics, Iowa State University. Vasant Honavar (PI), (2005-2007) \$25,000.
- 36. IGERT: Computational Molecular Biology Training Program. Vasant Honavar (Co-PI) with Dan Voytas (PI), Pat Schnable, Susan Carpenter, Jonathan Wendel (Co-Pis). National Science Foundation, 1999-2004., \$2,374,597 (plus \$1,161,010 in matching funds).
- 37. Developmental Proteomics of Retinal Progenitor Cells, National Institutes of Health (2003-2006). Vasant Honavar (Co-PI), (with Heather West-Greenlee and Jan Buss), \$438,000
- 38. NIH-NSF BBSI Summer Institute in Bioinformatics and Computational Biology Iowa State University. National Science Foundation, Vasant Honavar (Co-PI) with Volker Brendel (PI), Robert Jernigan, Karin Dorman, and Xun Gu (Co-Pis) (2002-2006). \$645,000.
- 39. Automated Integration of Condition Monitoring with an Optimized Maintenance Scheduler for Circuit Breakers and Power Transformers. Vasant Honavar (Co-PI) with James McCalley (PI) Mladen Kezunovic, and Chanan Singh (Co-Pis), Power Systems Engineering Research Center (a National Science Foundation Industry-University Research Center), 2002-2005. (2002-2005). \$255,000.
- 40. Symposium on Integration of Structural and functional Genomics, Vasant Honavar (co-PI) with Chris Tuggle (PI) and Marit Nielsen-Hamilton (Co-PI) National Science Foundation. (2005). \$10,900.
- 41. Exploring a Novel Proline Switch for Regulation of Protein Recognition. Center for Integrated Animal Genomics, Iowa State University, Vasant Honavar (Co-PI) with Drena Dobbs and Susan Carpenter (Co-Pis) (2004-2005) \$30,000.
- 42. Constructive Neural Network Learning Algorithms for Pattern Classification, National Science Foundation, 1994-1999, Principal Investigator, \$111,537 (plus \$10,000 in matching funds).
- 43. SGER: Multidisciplinary Aspects of Computation Theory, National Science Foundation, Vasant Honavar (Co-PI), with Jack Lutz (PI), Pavan Aduri (Co-PI), and Krishna Athreya (Co-PI), (2003- 2005). \$74,948.
- 44. Graduate Research Fellowships in Bioinformatics and Computational Biology, Pioneer Hi-Bred, Inc. 2002-2004. Major professor, Adrian Silvescu and Carson Andorf, \$80,000.
- 45. IBM Graduate Research Fellowship in Computer Science, IBM Inc., Major Professor, Doina Caragea, 2003-2004, \$30,000
- Interactive Visual Overviews of Large, Multi-Dimensional Datasets, Vasant Honavar (Co-PI) with Diane Cook (PI) and Les Miller (Co-PI) National Science Foundation, Co-Principal Investigator, 1999- 2003, \$370,000.
- Innovative Technologies for Defense Against Catastrophic Failures of Complex, Interactive Power Networks, U.S. Department of Defense (DOD) and Electric Power Research Institute (EPRI), \$4,500,000. (1999 – 2004) (Collaborative project involving 9 ISU faculty and faculty from 3 other universities). Co-Principal Investigator.

- 48. An Agent-Based System for Integration and Analysis of Distributed, Heterogeneous Plant Genome Databases. Pioneer Hi-Bred International, Inc., 2000-2002, Principal Investigator, \$40,000.
- 49. IBM Graduate Research Fellowship in Computer Science, IBM Inc., Vasant Honavar (Major Professor), with Doina Caragea (doctoral student), 2002-2003, \$30,000
- 50. Intelligent Multi-Agent Systems for Intrusion Detection, National Security Agency, 1998-2000, Co-Principal Investigator, \$199,769.
- 51. Data Mining of Electric Power Usage Data to Develop Customer Profiles. Cooperative Research Proposal. Power Domain, Inc. (2001-2002). Vasant Honavar. \$43,639.
- 52. SGER: Distributed Knowledge Networks to Support Security-Economy Decisions in Stressed Electric Power Systems. National Science Foundation, 2000-2001, Co-Principal Investigator, \$99,999.
- 53. Artificial Intelligence Applications to Power System Management and Control, Electric Power Research Institute, Co-principal investigator. 1998-2000, \$151,000
- 54. Distributed Knowledge Networks, John Deere Foundation, 1999-2001, Principal Investigator, \$30,000.
- 55. Development of Algorithmic Approaches to Gene Expression Analysis from Microarray Data, *Carver Foundation*, 2000-2001, Principal Investigator, \$25,000.
- 56. Development of Protein Structure Prediction Algorithms. Carver Foundation, 1999-2000, Co- Principal Investigator, \$25,000.
- 57. Genetic algorithms for protein structure prediction. Ames Laboratory, Co-Principal Investigator, 1999-2000. \$35,700.
- 58. A Gene-Specific DNA Chip for Exploring Molecular Evolutionary Change, *Carver Foundation*, 1998-1999. Co-Principal Investigator, \$17,120.
- 59. Intelligent Diagnosis Systems, John Deere Foundation, 1995-1998, Principal Investigator, \$30,000.
- 60. Graduate Fellowship (Data Mining and Knowledge Discovery), IBM Corporation, 1997-1998, Principal Investigator, \$20,800.

SELECTED RESEARCH PROJECTS AND RESEARCH ACCOMPLISHMENTS

Predictive models from ultra-high-dimensional longitudinal data (supported in part by the Huck Chair in Biomedical Data Sciences and Artificial Intelligence held by Vasant Honavar at Penn State University and grants from the NSF and NIH)

Longitudinal data, sometimes also called panel data, i.e., collections of repeated observations from a set of individuals, taken from a larger population, over time, often at irregularly spaced time points for everyone, are common across a broad range of applications, including health sciences, social sciences, learning sciences, economics, among others. Such data can be used to uncover the relationship between the time-varying patterns of certain measured variables (or features) and a particular outcome variable (or outcome) of interest, e.g., stock market crash, disease onset, health risk.

Longitudinal data exhibit longitudinal correlation (LC), i.e., correlations across observations of the same individual taken at different time points. In addition, observations across individuals may be correlated as well because of their shared traits (e.g., demographic characteristics), leading to clustered correlation (CC), or both. Under such circumstances, the observations (either within or across individuals) are no longer independent and identically distributed (i.i.d). Ignoring either part of the correlation can lead to incorrect parameter estimation, invalid tests of hypothesis, and misleading statistical inferences or predictions. Moreover, such data are characterized by fixed effects that are shared by the population under study; random effects that are individual-specific, or mixed effects, i.e., the combination of fixed effects and random effects. With the advent of big data, often the number of variables far exceeds the number of individuals, which increases the need for effective variable selection, computational efficiency,

and interpretable models. Last, but not the least, observations at any given time point have many missing measurements, and missing data are generally not missing at random.

Against this background, we are developing novel methods for predictive modeling from ultra-highdimensional, irregularly sampled, longitudinal data, including:

- Longitudinal Multi-Level Factorization Machines (LMLFM) (Liang et al., 2020), a novel, efficient, provably convergent extension of Factorization Machine (FM) for predictive modeling of longitudinal data characterized by mixed effects, in the presence of LC, CC, or both. A key feature of FM is that it models interactions of variables by mapping the interactions to dot products of vectors in a low dimensional latent space. LMLFM, like FM, uses latent factors to efficiently model higher order interactions between features. LMLFM extends FM to handle fixed, random, or mixed effects as needed for predictive modeling from longitudinal data. In addition, LMLFM incorporates a change in the structure of the underlying model to enhance model interpretability and achieve strictly linear training time with respect to the size of training data. To the best of our knowledge, LMLFM is the first multi-level regression model that extends variable selection beyond fixed effects to include random effects, and hence can be applied to high-dimensional longitudinal data. LMLFM uses a hierarchical probabilistic graphical model (HPGM) and avoids the need for hyperparameter tuning. LMLFM uses a variant of the iterated conditional modes (ICM) algorithm for learning the parameters of an LMLFM model based on a maximum a posteriori (MAP) formulation derived from the HPGM. We have established the convergence of LMLFM. Results of experiments with simulated data that show that LMLFM can effectively cope with high dimensional longitudinal data in the presence of both LC and CC whereas state-of-the-art baseline methods fail to do so (e.g., LMLFM can handle longitudinal data with over 5000 variables whereas the state-of-the-art baseline multilevel mixed effects models fail when the number of variables exceeds 100). Results of experiments with real-world data sets show that LMLFM compares favorably with the state-ofthe-art baselines in terms of predictive accuracy, while producing sparse, interpretable models that include only the relevant subset of variables.
- Longitudinal deep kernel Gaussian process regression (L-DKGPR) (Liang et al., 2021) to overcome these limitations by fully automating the discovery of complex multilevel correlation structure from longitudinal data. Specifically, L-DKGPR eliminates the need for ad hoc heuristics or trial and error using a novel adaptation of deep kernel learning that combines the expressive power of deep neural networks with the flexibility of non-parametric kernel methods. L-DKGPR effectively learns the multilevel correlation with a novel additive kernel that simultaneously accommodates both time-varying and the time-invariant effects. We have developed an efficient algorithm to train L-DKGPR using latent space inducing points and variational inference. Results of extensive experiments on several benchmark data sets demonstrate that L-DKGPR significantly outperforms the state-of-the-art longitudinal data analysis (LDA) methods.
- A novel, modular, convolution-based feature extraction and attention mechanism that simultaneously identifies the variables and time intervals over which the variables identified impact the classifier output (Hsieh et al., 2021). The results of our extensive experiments with several benchmark data sets that show that the proposed method outperforms the state-of-the-art baseline methods on multi-variate time series classification task. The results of our case studies demonstrate that the variables and time intervals identified by the proposed method make sense relative to available domain knowledge.
- Functional autoencoders (Hsieh et al., 2021), which generalize neural network autoencoders to learn non-linear representations of functional data. We have derived from first principles, a functional gradient based algorithm for training functional autoencoders. The results of experiments demonstrate that the functional autoencoders outperform the state-of-the-art baseline methods. The resulting methods find applications in many real-world settings, e.g.,

monitoring of individual health, climate, brain activity, environmental exposures, among others, the data of interest change smoothly over a continuum, e.g., time, yielding multi-dimensional functional data. Functional data representations can be used for functional data clustering, classification, and regression.

• SRVAR (Hsieh et al., 2021), a novel approach to the problem of simultaneously learning the dynamics of transitions between hidden states and the state-dependent relationships between variables. SRVAR uses state space recurrent neural networks to model the transitions between hidden states and utilizes the smooth acyclic characterization of DAGs to efficiently learn the state-dependent DAGs. We have results of experiments on simulated data as well as a real-world data set that show the superiority of SRVAR over state-of-the-art baselines in recovering the patterns of state transitions while modeling state-specific dependencies between variables.

Continual Learning (Funded in part by the National Science Foundation and the Huck Chair in Biomedical Data Sciences and Artificial Intelligence held by Vasant Honavar). Continual learning refers to the problem of acquiring new information as new data, new classes, or new tasks are presented over time. One of the goals of CL is to maintain performance on previously learned classes or tasks while effectively leveraging previously acquired knowledge to perform well on the new data, classes, or tasks: (i) task-incremental learning where the goal is to incrementally learn a set of clearly distinguishable tasks; (ii) domain-incremental learning which is a more challenging case of task-incremental learning where the goal is to incrementally learn to distinguish between a growing number classes. In many applications, it is necessary to consider the regression counterpart of CIL.

Existing CL methods have several significant limitations: (i) CL methods have been evaluated primarily on limited computer vision benchmark data, on which some very simple baseline CL methods have been shown to work well; (ii) Different CL methods often make different assumptions, making it hard to rigorously compare them; (iii) The surprisingly good performance of simple baselines on commonly used benchmarks calls into question the adequacy of the benchmarks, the current state of progress on CL, or both; (iv) Barring a few exceptions, there are few theoretical guarantees about the performance of most CL algorithms; and (v) CL methods generally fail to explicitly consider the costs of storing and processing old data, the learned model, or the cost of adapting a learned model to a new task. Hence, there is an urgent need for rigorous formulations of CL problems, CL algorithms with strong performance guarantees, and better benchmarks for rigorous evaluation. Our recent work has led to:

- A simple, fast algorithm inspired by adaptive resonance theory (ART) (Ashtekar et al., 2023). To cope with the curse of dimensionality and avoid catastrophic forgetting, we apply incremental principal component analysis (IPCA) to the model's previously learned weights. Experiments show that this approach approximates the performance achieved using static PCA and is competitive with continual deep learning methods.
- A new method for efficient continual learning of sparse models (EsaCL) that can automatically
 prune redundant parameters without adversely impacting the model's predictive power and
 circumvent the need of retraining (Ren et al., 2024). Based on a theoretical analysis of loss
 landscapes we design directional pruning (SDP) strategy that is informed by the sharpness of
 the loss function with respect to the model parameters. SDP ensures model with minimal loss
 of predictive accuracy, accelerating the learning of sparse models at each stage. To accelerate
 model update, we use a data selection strategy to identify critical instances for estimating loss
 landscape. The results of our experiments show that EsaCL achieves performance that is
 competitive with the state-of-the-art methods.

Work in progress is aimed at (i) investigating the necessary and sufficient conditions for CL problems to be solvable; (ii) formulating CL problems as optimization problems to model the relevant costs and derive

CL solutions with strong performance guarantees; and (iii) developing physics-based formulations of CL where the tasks and data change, but the governing physics does not.

Hyperdimensional Representations (Funded in part by grants from the National Science Foundation and the National Institutes of Health). Recent years have seen unprecedented advances in deep learning algorithms for a variety of applications including computer vision, natural language processing, multimodal representation learning, node labeling and link prediction in social networks, molecular structure classification, among others. However, such methods are data hungry, require extensive hyperparameter tuning, and achieve their superior performance at considerable computational cost, resulting in a large carbon footprint with attendant adverse environmental impacts. Hence, there is an urgent need for computationally efficient and consequently, environmentally more sustainable alternatives to deep learning across a broad range of AI applications.

Against this background. We explore hyperdimensional computing as a brain-inspired alternative to deep neural networks for artificial intelligence and machine learning applications. Hyperdimensional representation maps each object using a sufficiently high-dimensional random encoding to produce a binary or bipolar vector. All computations are performed on the objects thus encoded using simple operations, e.g., element-wise additions and dot products. Computations on HD vectors, because they yield binary or bipolar vectors, can be realized using low-precision, fast, low-power, energy-efficient hardware. Our recent work has resulted in:

- A Hyper-dimensional Graph Learning (HDGL) algorithm. HDGL leverages the injectivity property of node representations of a family of Graph Neural Networks (GNNs) to map node features to the HD space and then uses HD operators such as bundling and binding to aggregate information from the local neighborhood of each node. The resulting latent node representations support both node classification and link prediction tasks, unlike typical deep learning methods, which often require separate models for these tasks. The results of our experiments using widely used benchmark datasets which demonstrate that, on the node classification task, HDGL yields performance that is competitive with the state-of-the-art GNN methods at substantially reduced computational cost. Furthermore, HDGL is well-suited for class incremental learning where the model has to learn to effectively discriminate between a growing number of classes. Our experiments also show that the HD representation constructed by HDGL supports link prediction at accuracies comparable to that of DeepWalk and related methods. Thus, HDGL offers a computationally efficient alternative to graph neural networks for node classification, especially in settings that call for class-incremental learning or in applications that demand high accuracy models at significantly lower computational cost and learning time than possible with the state-of-the-art graph neural network methods.
- A hyper-dimensional causal effect estimation method. Matching is one of the simplest approaches for estimating causal effects from observational data. Matching techniques compare the observed outcomes across pairs of individuals with similar covariate values but differing in their treatment status in order to estimate causal effects. However, traditional matching techniques are unreliable when faced with high-dimensional covariates due to the infamous curse of dimensionality. To overcome this challenge, we propose a simple, fast, yet highly effective approach to matching using Random Hyperplane Tessellations (RHPT). We prove that the RHPT representation is an approximate balancing score thus maintaining the strong ignorability assumption and provide empirical evidence for this claim. We report results of extensive experiments showing that matching using RHPT outperforms traditional matching techniques and is competitive with state-of-the-art deep learning methods for causal effect estimation. In addition, RHPT avoids the need for computationally expensive training of deep neural networks.

Generative Models for Complex Data (Funded in part by grants from the National Science Foundation and the National Institutes of Health). Generative models trained on large data sets have had astounding

success at text, image, video, and even molecular structures. We are developing computationally efficient yet accurate learning algorithms for a variety of applications of generative models. Our recent work has resulted in:

- GraphECL, a simple contrastive learning algorithm for fast and accurate inference on graphs. Graph contrastive learning offers a promising approach to applications where there is a scarcity of task-specific labels. However, existing methods for graph contrastive learning incur significant computational overhead for due to their reliance on message passing. This makes them unsuitable for latency-constrained applications. GraphECL does away with the need for expensive message passing during inference. It introduces a novel coupling of the MLP and GNN models, where the former learns to computationally efficiently mimic the computations performed by the latter. We provide a theoretical analysis showing why MLP can capture essential structural information in neighbors well enough to match the performance of GNN in downstream tasks. Extensive evaluations using widely used real-world benchmarks that show that GraphECL achieves superior performance and inference efficiency compared to state-of-the-art graph contrastive learning (GCL) methods on homophilous and heterophilous graphs.
- Foundation models trained on large data sets of molecules (e.g., proteins, material structures) have proven useful for applications such as drug discovery and material discovery. Generative models trained on molecular structures are quite effective at capturing structural information about the molecules. However, they fail to take advantage of rich information available in textual descriptions of the molecular properties, or information available through other modalities. Hence, we extract and curate 200,000 pairs of molecular structures and their descriptions taken from biomedical texts to obtain the PubChem3D dataset. We use generative models trained on the resulting data set to demonstrate superior performance on several tasks including molecular property prediction, zero-shot text-guided molecule retrieval, and 3D molecule description.
- A multi-modal representation learning framework over natural language text, chemical descriptions
 of molecules, 3D binding pockets, among others. To facilitate direct experimental evaluation of the
 resulting framework, we assembled a high-quality data set. We trained and evaluated a multimodal
 generative model on several cross-modal retrieval tasks: Molecule to Language (M2L), Language
 to Molecule (L2M), Language to Conformation (L2C), and Conformation to Language (C2L).

Work in progress is aimed at incorporating physics into large-scale data-driven generative models, including those for materials discovery and drug design.

Knowledge-based Machine Learning (Funded in part by grants from the National Science Foundation and the Huck Chair in Biomedical Data Sciences and Artificial Intelligence). Scientific applications of machine learning present a growing need for incorporating physics, constraints, e.g., symmetries, invariances, equivariances, measurement uncertainties, process descriptions, e.g., differential equations, algebraic functional forms, knowledge graphs, e.g., periodic table of elements, to overcome the limitations of otherwise purely data-driven ML models. Existing knowledge-informed ML (KIML) methods fall into the following : (i) Physics-informed ML (PIML) methods that incorporate physics into ML, e.g., neural network architecture or loss function; (ii) Methods that incorporate domain knowledge as constraints or terms in the objective function; (iii) Geometric learning methods that ensure that incorporate invariances, and equivariances into learned representations; and (iv) Bayesian models that incorporate knowledge into priors. Our recent work has resulted in:

- Methods that exploit knowledge of the periodic table to adapt machine learned interatomic potentials to new material structures made of elements that do not appear in the training data.
- Knowledge-based extensions of the state-of-the-art physics-based reactive force-field pioneered by van Duin with additional parameterized functional obtaining significant improvements the state-of-the-art methods in accuracy as well as speed. This approach could vastly make high-accuracy potential based reactive MD simulations more accessible to a broader range of researchers.

Work in progress aims to develop generalizable approaches to informing data driven machine learning methods with knowledge of various forms, and evaluating the resulting methods on scientific applications, e.g., construction of universal interatomic potentials and thermodynamic equations for materials discovery, design, and synthesis.

Predictive and Causal Modeling of Health Outcomes from Clinical, Behavioral, Biomedical, Socio-Demographic, and Environmental Data (Funded in part by grants from the National Science Foundation and the National Institutes of Health). There is increasing recognition that environmental and contextual factors can have a significant impact on the health outcomes in diseases such as cancer, obesity, diabetes, heart disease. The advent of "big data" offers enormous potential for understanding and predicting health risks, intervention outcomes, and personalized treatments, ultimately improving population health through integrative analysis of heterogeneous, fine-grained, richly structured, longitudinal patient data. This project aims to bring together an interdisciplinary team of researchers to understand the clinical, behavioral, biomedical environmental, and contextual (e.g., socio-demographic) factors that contribute to increased risk of specific diseases, e.g., breast cancer; and developing evidencebased practices for supplemental screening, as well as behavioral or clinical interventions to mitigate the risk. The project leverages the Digital Precision Health Collaboratory, which offers secure infrastructure for data access and use policy compliant EHR data coded using standardized vocabularies. The key methodological and informatics innovations in the project have to do with the development of novel algorithms and tools for predictive modeling of health risks and health outcomes by integrating clinical, biomedical, environmental, socio-demographic, and behavioral data. Work in progress is aimed at:

- Developing predictive models of health risks and intervention outcomes from selected environmental, behavioral, biomedical, socio-demographic data
- Developing causal models of health risks and intervention outcomes from selected environmental, behavioral, biomedical, socio-demographic data
- Eliciting the environmental, contextual, behavioral, health status and health care factors that are reliable predictors of health disparities through integrative analysis of clinical, environmental, behavioral, biomedical, socio-demographic data.

Causal Inference from Observational and Experimental Data (supported in part by Huck Chair in Biomedical Data Sciences and Artificial Intelligence held by Vasant Honavar and a grant from the National Science Foundation). Elicitation of a causal effect from observations and experiments is central to scientific discovery, or more generally, rational approaches to understanding and interacting with the world around us. Judea Pearl introduced causal diagrams provide a formal representation for combining data with causal information and do-calculus to provide a sound and complete inferential machinery for causal inference.

The practical need to transfer causal effects elicited in one domain (setting, environment, population) e.g., a controlled laboratory setting, to a different setting presents us with the problem of transporting causal information from a source environment to a different target environment. For example, one might want to know if causal relation between teaching strategies and student learning obtained by through a randomized trial in a public school in Chicago can be transported to a public school in Minneapolis that has an admittedly different population of students. Our recent work has led to theoretical characterization and algorithms for:

(a) *m*-transportability, a generalization of transportability, which offers a license to use causal information elicited from experiments and observations in *m* (where *m* is greater than or equal to 1) source settings to estimate a causal effect in each target setting. We have established the necessary and sufficient conditions for *m*-transportability. We have designed an algorithm for deciding *m*-transportability that determines whether a causal relation is m-transportable; and if it

is, produces a transport formula, that is, a recipe for estimating the desired causal effect by combining experimental information from m source environments with observational information from the target environment (Lee et al., 2013)

- (b) *z*-transportability, the problem of estimating the causal effect of a set of variables X on another set of variables Y in a target domain from experiments on any subset of controllable variables Z where Z is an arbitrary subset of observable variables V in a source domain. Z-Transportability generalizes *z*-identifiability, the problem of estimating in each domain the causal effect of X on Y from surrogate experiments on a set of variables Z such that Z is disjoint from X. *z*- Transportability also generalizes transportability which requires that the causal effect of X on Y in the target domain be estimable from experiments on any subset of all observable variables in the source domain. We have generalized z-identifiability to allow cases where Z is not necessarily disjoint from X. We have established a necessary and sufficient condition for z-transportability in terms of generalized zidentifiability and transportability. We have provided a sound and complete algorithm that determines whether a causal effect is z-transportable; and if it is, produces a transport formula, that is, a recipe for estimating the causal effect of X on Y in the target domain using information elicited from the results of experimental manipulations of Z in the source domain and observational data from the target domain. Our results also show that do-calculus is complete for z-transportability (Lee et al., 2013).
- (c) *mz*-transportability, the problem of inferring a causal effect of treatment variables on observables in a target domain (environment, experimental setting) by combining data from experiments on simultaneously controllable subsets of variables (together with observations) from multiple domains (including the target domain). We have provided an efficient and complete algorithm that determines if a causal effect is mz-transportable, and if so, outputs a transport formula for estimating the causal effect. These results set the stage for considering more general forms of meta-identifiability by allowing a fully arbitrary information set and for proving the completeness of do-calculus in such settings (Bareinboim et al., 2013).

We have examined the following problem in causal inference: Given a causal graph G, determine MIC(G), that suffices for identifying every causal effect that is identifiable in a causal model characterized by G. We have established the completeness of do-calculus for computing MIC(G). MIC(G) effectively offers an efficient compilation of all the information obtainable from all possible interventions in a causal model characterized by G. Minimum intervention cover finds applications in a variety of contexts including counterfactual inference, and generalizing causal effects across experimental settings. We analyze the computational complexity of minimum intervention cover and identify some special cases of practical interest in which MIC(G) can be computed in time that is polynomial in the size of G.

Work in progress is aimed at (i) bridging the gap between theory and practice of causal inference to address the needs of real-world applications, e.g., by developing algorithms and software for eliciting causal effects from temporal and temporal-relational data.

Relational Causal Models (funded in part by a grant from the National Science Foundation). Most work on causal inference from observational data has assumed that the observations are independent and identically distributed. However, in many practical applications, the data exhibit relational dependencies. Relational causal models (RCM) allow us to model causal relationships in relational data. Our recent work has led to:

(a) A characterization of the properties of abstract ground graphs (AGG), which play a key role in the proofs of completeness of the only previous algorithm for learning relational causal models from data, we showed that AGG representation is not complete for relational *d*-separation, that is, there can exist conditional independence relations in an RCM that are not entailed by AGG (Lee et al., 2015).

- (b) An investigation of Relational Causal Models (RCM) under relational counterparts of adjacencyfaithfulness and orientation-faithfulness, yielding a simple approach to identifying a subset of relational *d*-separation queries needed for determining the structure of an RCM using *d*separation against an unrolled DAG representation of the RCM. We provided theoretical underpinnings of a basis of a sound and efficient algorithm for learning the structure of an RCM from relational data. We introduced RCD-Light, a sound and efficient constraint-based algorithm that is guaranteed to yield a correct partially directed RCM structure with at least as many edges oriented as in that produced by RCD, the only other existing algorithm for learning RCM. We showed that unlike RCD, which requires exponential time and space, RCD- Light requires only polynomial time and space to orient the dependencies of a sparse RCM (Lee et al., 2016).
- (c) A novel and elegant characterization of the Markov equivalence of RCMs under *path semantics, an alternative to bridge-burning semantics used by RCD.* We introduced a novel representation that allows us to efficiently determine whether an RCM is Markov equivalent to an-other. Under path semantics, we provide a sound and complete algorithm for recovering the structure of an RCM from conditional independence queries. Our analysis also suggests ways to improve the orientation recall of algorithms for learning the structure of RCM under *bridge burning semantics* as well (Lee et al., 2016).

Federated Data and Computational Infrastructure for Collaborative, Data-Intensive Science

(funded in part by a grant from the National Science Foundation). Scientific progress in many disciplines is increasingly enabled by our ability to examine natural phenomena through the computational lens (e.g., using algorithmic abstractions of the underlying processes) and our ability to acquire, share, integrate, and analyze disparate types of data. However, realizing the full potential of data to accelerate science calls for significant advances in data and computational infrastructure to support collaborative data-intensive science by teams of researchers that transcend institutional and disciplinary boundaries.

This project aims to conceptualize, design, and implement a Virtual Data Collaboratory (VDC), to support collaborative, data-intensive science research by multi-disciplinary teams drawn from multiple institutions. Specifically, the project aims to design VDC, a federated infrastructure that integrates the state-of-the-art data-intensive computing platforms, storage, and networking, with an innovative data services layer across Rutgers University, Pennsylvania State University, and several other institutions in the region, interconnected through a high-speed network, with the potential to expand to incorporate academic/research institutions across the United States. VDC will leverage existing national/international and regional data repositories (including NSF funded repositories like the Ocean Observatories Initiative (OOI) and the Protein Data Bank (PDB)), existing investments in advanced cyberinfrastructure, like the NSF funded Big Data Regional Hubs, XSEDE, OSG, among others.

VDC will provide the collaborative infrastructure and platform for developing and integrating algorithmic abstractions of scientific domains e.g., biology, coupled with methods and tools for data analytics, modeling, and simulation, cognitive tools (representations, processes, protocols, workflows, software) to advance science. VDC will support reproducible, sharable, and reconfigurable data- intensive scientific workflows [Parashar et al., 2019].

The project will use several collaborative science use cases to develop and evaluate the VDC infrastructure. For example, one use case involves a collaboration between Vasant Honavar and Helen Berman, a Rutgers structural biologist and the founder of the Nucleic Acid Database (NDB) and former director of the Protein Data Bank (PDB), a widely used archival database of curated protein structures, will use VDC to assemble carefully curated data sets of protein-DNA and protein RNA complexes and interfaces; and develop machine learning and other computational methods and tools for reliable prediction of protein-RNA and protein-DNA interfaces. The team will use VDC to establish shared data and computational infrastructure, complete with workflows for documenting, comparing, and

reproducing computational analyses and prediction of protein-RNA complexes, interfaces. In addition to helping develop and evaluate the VDC infrastructure, the results of this effort will advance our understanding of the molecular mechanisms by which proteins recognize and bind to DNA and RNA, and their role in a variety of important biological processes that orchestrate development, aging, disease, etc.

Algorithms and Software for Knowledge Acquisition from Semantically Heterogeneous,

Distributed Data (funded in part by grants from the National Science Foundation)

The emergence of big data offers unprecedented opportunities in knowledge acquisition (e.g., discovery of a priori unknown complex relationships, construction of predictive models) from data. However, realizing these opportunities in practice presents several challenges. Data repositories are autonomously designed and operated, large, physically distributed, and differ in structure, organization, semantics, and query and processing capabilities. Our research, aimed at addressing some of these challenges, has led to:

- (a) The development of a general theoretical framework for learning predictive models (e.g., classifiers) from large, physically distributed data sources where it is neither desirable nor feasible to gather all the data in a centralized location for analysis. This framework (Caragea et al., 2001; 2003; 2004a) offers a general recipe for the design of algorithms for learning from distributed data that are *provably exact* with respect to their centralized counterparts (in the sense that the model constructed from a collection of physically distributed data sets is provably identical to that obtained in the setting where the learning algorithm has access to the entire data set). A key feature of our approach is the clear separation of concerns between hypothesis construction and extraction and refinement of *sufficient statistics* needed by the learning algorithm from data which reduces the problem of learning from data to a problem of decomposing a query for sufficient statistics across multiple data sources and combining the answers returned by the data sources to obtain the answer for the original query. Our work has resulted in provably exact algorithms (relative to the centralized counterparts) for learning a variety of predictive models from distributed data.
- (b) The development of theoretically sound yet practical variants of a large class of algorithms (Caragea et al., 2001; 2003; 2004a; Koul et al., 2010; Lin et al., 2011; 2013) for learning predictive models (classifiers) from distributed data sources under a variety of assumptions (motivated by practical applications) concerning the nature of data fragmentation, and the query capabilities and operations permitted by the data sources (e.g., execution of user supplied procedures), and precise characterization of the complexity (computation, memory, and communication requirements) of the resulting algorithms relative to their centralized counterparts.
- (c) The development of a theoretically sound approach to formulation and execution of statistical queries across semantically heterogeneous data sources (Caragea et al., 2004b; Caragea et al., 2005; Caragea et al., 2006; 2007; 2010). This work has shown how to use semantic correspondences and *mappings* specified by users from a set of terms and relationships among terms (user ontology) to terms and relations in data source specific ontologies to construct a sound procedure for answering queries for *sufficient statistics* needed for learning classifiers from semantically heterogeneous data. An important component of this work is the development of statistically sound approaches to handling data specified at different levels of abstraction across different data sources (Zhang et al., 2003, 2006).
- (d) Abstraction-Driven Algorithms for Building Compact yet Accurate Classifiers. We have developed a general approach for exploiting attribute value hierarchies (AVH) that group the values of attributes to learn compact yet accurate predictive models from data specified at different levels of abstraction. Instantiations of this approach in the case of Naïve Bayes (Zhang et al., 2004; 2006), Decision Trees (Zhang et al., 2003), and Markov Models (Caragea et al., 2010) show that the resulting algorithms

yield predictive models that are more compact than those produced by their counterparts that do not have access to AVH without sacrificing the quality of the predictors.

- (e) Demonstration of the theoretical equivalence of a certain class of inter-ontology mapping errors and noise models, and hence the reduction of the problem of learning in the presence of mapping errors from semantically disparate data to the problem of learning from noisy data (Koul et al., 2010, 2012).
- (f) The design and implementation of INDUS A modular, extensible, open-source software toolkit for data-driven knowledge acquisition from large, distributed, autonomous, semantically heterogeneous data sources¹².

Research in progress is aimed at:

- (a) Extension of the statistical query-based learning framework to learning predictive models from Linked Open (RDF) Data e.g., algorithms for learning Relational Bayesian Classifiers from RDF data in settings where the learner can access the RDF data only through a restricted set of queries against an access interface (Lin et al., 2011).
- (b) Extension of the statistical query-based learning framework to learning predictive models from network data

Applications of the resulting algorithms to social network and social media analytics and analysis and prediction of biomolecular interaction.

Learning Predictive Models from Richly Structured Data

Learning Predictive Models from Partially Specified, Sparse Data: Many applications, e.g., medical diagnosis, different cases may be described in terms of symptoms or results of diagnostic tests are only partially specified e.g., a patient may be described as having cardiac arrhythmia without specifying the precise type of arrhythmia. Other applications present the problem of learning predictive models from sparse data, e.g., each patient exhibits only a small subset of symptoms. My students and I pioneered a principled approach to learning compact yet accurate predictive models from data specified at varying levels of precision or abstraction and demonstrated how the approach could be used to learn accurate, and compact (and hence easy-to-comprehend) predictive models from sparse data, noisy data. The resulting methods have found applications in bioinformatics, health informatics, and social informatics. Some results of this work include:

- (a) Abstraction Augmented Markov models (AAMMs). AAMMs are generalizations of Markov Models (MM). AAMMs simplify the data representation used by the standard MMs by grouping similar subsequences to organize them in an abstraction hierarchy (Caragea et al., 2010a, 2010b, 2010c). Experimental results on text document classification and protein subcellular localization show that adapting data representation by combining super-structuring and abstraction makes it possible to construct predictive models that use much fewer features (by one to three orders of magnitude) than those obtained using super-structuring alone (whose size grows exponentially with the length of direct dependencies). Super-structuring and abstraction-based models are competitive with and, in some cases, outperform, models that use only super- structuring. Our experiments have also demonstrated the promise of abstraction-augmented Markov Models in learning sequence classifiers in a semisupervised setting where only some of the sequences are labeled.
- (b) Development of Abstraction-super-structuring Normal Forms (Silvescu and Honavar, 2011) that offer a general theoretical framework for structural (as opposed to parametric) aspects of induction using abstraction (grouping of similar entities) and super-structuring (combining topologically close entities) and exploration of its relation to ideas e.g., radical positivism in the philosophy of science (with PhD

¹ <u>http://code.google.com/p/induslearningframework/</u>

² <u>http://code.google.com/p/indusintegrationframework/</u>

student Adrian Silvescu).

(c) Development of methods for taking advantage of abstractions to build compact yet accurate predictive models for labeling actors in social networks (Bui et. Al., 2013) and for building predictive models RDF data by taking advantage of RDFS hierarchies (Lin et al., 2015).

Work in progress is aimed at extending this approach to learning predictive models from richly structured data at multiple levels of abstraction (images and text (multi-modal data), social networks and social media, linked open data, biomolecular interaction network data).

Learning Predictive Models from Multi-Modal, Multi-View Data

Recent years have witnessed rapid advances in our ability to acquire and store massive amounts of data across different modalities (such as text, speech, images, etc. on the web; genomics, transcriptomics, proteomics, metabolomics data in life sciences; fMRI, diffusion tensor imaging, etc. in brain sciences; Different types of digital objects e.g., movies, music, etc. associated with individuals in a social network). Some of this work also had to cope with the challenges presented by the limited availability of labeled data, and the need for accommodating multiple labels for data instances. We have developed multimodal machine learning algorithms for image annotation, the task of assigning keywords to an image based on its contents, labeling actors in social networks (e.g., with respect to their interest in specific content, e.g., movies, music, etc.). Some results of this work include:

- (a) Multimodal Hierarchical Dirichlet Process Models, non-parametric generalizations of the hierarchical mixture models. Our experimental evaluation shows that the performance of this model does not depend on the number of mixture components, unlike the standard mixture model which suffers from over-fitting (Yakhnenko and Honavar, 2009).
- (b) Formulation of image annotation as a multiple instance, multiple label learning problem, which is a generalization of supervised learning in which the training examples are bags of instances, and each bag is labeled with a set of labels. We learn as many classifiers as there are possible labels and force the classifiers to share weights using trace-norm regularization. Our experimental results on standard benchmark datasets show that the performance of this model is comparable to the state- of-the-art multiple instance multiple label classifiers and that unlike some state-of-the-art models, it is scalable and practical for datasets with many training instances and labels (Yakhnenko and Honavar, 2011).
- (c) A generalization of the discriminative model to a semi-supervised setting to allow the model take advantage of labeled and unlabeled data. We assume that the data lies in a low-dimensional manifold and introduce a penalty that ensures that the classifiers assign similar labels to similar instances (i.e. instances that are near-by in the manifold induced by the samples). Our experimental results show the effectiveness of this approach in learning to annotate images from partially labeled data (Yakhnenko and Honavar, 2010).
- (d) A novel kernel-based approach for predicting labels of actors in multi-view social networks. Here, given a social network in which only a subset of the actors is labeled, our goal is to predict the labels of the rest of the actors. We introduced a new random walk kernel, namely the Inter-Graph Random Walk Kernel (IRWK), for labeling actors in multi-view social networks. IRWK combines information from within each of the views as well as the links across different views that outperform or are competitive with several state-of-the-art methods for labeling actors in social networks (Bui et al., 2016).
- (e) A novel use of knowledge graphs, that capture general or commonsense knowledge, to augment the information extracted from images by the state-of-the-art methods for image captioning. The results of our experiments, on several benchmark data sets such as MS COCO, as measured by CIDEr-D, a performance metric for image captioning, show that the variants of the state-of-the- art methods for image captioning that make use of the information extracted from knowledge graphs can substantially outperform those that rely solely on the information extracted from images (Zhou et image captor)

al., 2019).

- (f) A novel multi-view network embedding (MVNE) algorithm for constructing low-dimensional node embeddings from multi-view networks. MVNE adapts and extends an approach to single view network embedding (SVNE) using graph factorization clustering (GFC) to the multi-view setting using an objective function that maximizes the agreement between views based on both the local and global structure of the underlying multi-view graph. Our experiments with several benchmark real-world single view networks show that GFC-based SVNE yields network embeddings that are competitive with or superior to those produced by the state-of-the-art single view network embedding methods when the embeddings are used for labeling unlabeled nodes in the networks. Our experiments with several multi-view networks show that MVNE substantially outperforms the single view methods on integrated view and the state-of-the-art multi-view methods. We further show that even when the goal is to predict labels of nodes within a single target view, MVNE outperforms its single-view counterpart suggesting that the MVNE can extract the information that is useful for labeling nodes in the target view from all the views (Sun et al., 2018).
- (g) A novel optimization algorithm for y machine learning, and statistical inference problems that call for minimization of a composition of expected value functions (CEVF). We have introduced compositional stochastic average gradient descent (C-SAG) a novel extension of the stochastic average gradient method (SAG) to minimize composition of finite-sum versions of such compositional optimization problems. C-SAG, like SAG, estimates gradient by incorporating memory of previous gradient information. We have presented detailed theoretical analyses of C- SAG which show that C-SAG, like C-SVRG, achieves a linear convergence rate for strongly convex objective function; However, C-CAG achieves lower oracle query complexity per iteration than C- SVRG. Our experiments show that C-SAG converges much faster than full gradient (FG) and C-SVRG (Hsieh et al., 2018).

Work in progress is aimed at developing efficient methods for learning accurate predictive models from multi-modal data, including data available at various levels of granularity or abstraction, across a broad range of applications, including predictive modeling of health outcomes and disease phenotypes from behavioral, clinical, biomedical, environmental, and socio-demographic data.

Topics in Grammar Inference and Computational Learning Theory

Grammatical Inference, variously referred to as automata induction, grammar induction, and automatic language acquisition, refers to the process of learning of grammars and languages from data. Machine learning of grammars finds a variety of applications in syntactic pattern recognition, adaptive intelligent agents, diagnosis, computational biology, systems modeling, prediction, natural language acquisition, data mining and knowledge discovery.

Our work on learning Regular Grammars demonstrates the feasibility of learning regular languages from examples under additional assumptions concerning the distribution from which the examples are drawn, thereby addressing the problem ("Are DFA PAC-identifiable if examples are drawn from the uniform distribution, or some other known simple distribution?") posed by Pitt in his seminal paper (against the background of strong negative results regarding the feasibility of learning regular grammars within the standard PAC learning framework):

- a) The class of simple DFA (i.e., DFA whose canonical representations have logarithmic Kolmogorov complexity) is efficiently PAC learnable under the Solomonoff Levin universal distribution (Parekh and Honavar, 1999).
- b) If the examples are sampled at random according to the universal distribution by a teacher that is knowledgeable about the target concept, the entire class of DFA is efficiently PAC learnable under the universal distribution, that is, DFA are efficiently learnable under the PACS Model (Parekh and Honavar, 1999; Parekh and Honavar, 2001).

c) Any concept that is learnable under Gold's model for learning from characteristic samples, Goldman, and Mathias' polynomial teachability model, and the model for learning from examplebased queries is also learnable under the PACS model (Parekh and Honavar, 2000; 2001).

Related work has led to the development of polynomial algorithms for learning regular languages from examples and membership queries (Nichitiu et al., 2000).

Our work on learning of grammars used to model natural languages (in particular, dependency grammars, stochastic context free grammars) has led to:

- (a) The development of a novel regularization scheme, namely, unambiguity regularization that favors grammars that yield unambiguous parses, which includes as special cases and improves upon, standard expectation maximization (EM), Viterbi EM, and Softmax EM algorithms for unsupervised learning of grammars (Tu and Honavar, 2012).
- (b) Demonstration (and explanation) of the benefits of *curricula* (e.g., a means of ordering training samples presented to the learner in an inductive learning setting) using an incremental construction hypothesis which asserts (loosely speaking) that when the target of learning is a structure e.g., a grammar that can be decomposed into a set of sub-structures e.g., grammar rules, an ideal curriculum is one that gradually emphasizes data samples that help the learner to successively discover new substructures (Tu and Honavar, 2011).
- (c) An iterative bi-clustering approach to learning probabilistic context free grammars (Tu et al., 2008, 2011).

Work in progress is aimed at extending the theoretical foundations and algorithms for grammar inference to settings that call for learning from multimodal data (e.g., combination of words and pictures). Some results to date include an algorithm for learning a multi-modal hierarchical Dirichlet process model for annotating images from partially labeled data (Yakhnenko and Honavar, 2009).

Explaining Machine Learned Predictive Models and their predictions (funded in part by a grant from the NSE)

from the NSF)

Our ability to acquire and annotate increasingly large amounts of data together with rapid advances in machine learning have made predictive models trained using machine learning ubiquitous in virtually all areas of human endeavor. In high-stakes applications such as healthcare, finance, criminal justice, scientific discovery, education, and others, the resulting predictive models are complex, and in many cases, blackboxes. Consider for example, a medical decision-making scenario where a predictive model, e.g., a deep neural network, trained on a large database of labeled data, is to assist physicians in diagnosing patients. In this setting, it is important that the clinical decision support system be able to explain the output of the deep neural network to the physician, who may not have a deep understanding of machine learning. For example, the physician might want to understand the subset of patient characteristics that contribute to the diagnosis; or the reason as to why diagnoses were different for two different patients, etc. In high stakes applications of machine learning, the ability to explain the machine learned model is a prerequisite for establishing trust in the model's predictions. Satisfactory explanations must provide answers to questions such as: "What features of the input are responsible for the predictions?" "Why are the model's outputs different for two individuals?" (e.g., Why did John's loan application get approved when Sarah's was not?). Hence, satisfactory explanations must be fundamentally causal in nature. This project aims to develop a theoretically sound, yet practical approach to causal attribution, that is, apportioning the responsibility for a black-box predictive model's outputs among the model's inputs.

We reduce the model interpretation question "Why did the predictive model generate the output Y for input X?" to the following equivalent question: "How are the features of the model input X causally related to the model output Y?" In other words, we reduce the task of interpreting a black-box predictive model to the

task of estimating, from observations of the inputs and the corresponding outputs of the model, the causal effect of each input variable or feature on the output variable. Our methods do not require knowledge of the internal structure or parameters of the black-box model, or of the objective function or the algorithm used to train the model. Hence, the resulting methods can be applied, in principle, to any black-box predictive model, so long as it is possible to probe the model and observe the model's response to any supplied input data sample.

Federated Ontologies Knowledge Representation and Inference (funded in part by a grant from the National Science Foundation)

The success of the world wide web can be attributed to the *network effect*: The absence of central control on content and organization of the web allows thousands of independent actors to contribute resources (web pages) that are interlinked to constitute the web. Recent efforts to extend the web into a *semantic web* are aimed at enriching the web with machine interpretable content and interoperable resources and services. Realizing the full potential of the semantic web requires the large-scale adoption and use of ontology-based approaches to sharing of information and resources. In such a setting, instead of a single, centralized ontology, it is much more natural to have a federation of ontologies that cover different, partially overlapping, domains (e.g., biology, medicine, pharmacology). Such ontologies represent the *local* knowledge of the ontology designers, that is, knowledge that is applicable within a specific *context*. Hence, there is an urgent need for theoretically sound yet practical approaches that support user, context, or application-specific adaptation and reuse of knowledge from multiple autonomously developed ontologies in specific applications. Ontologies on the semantic web need to satisfy conflicting objectives: Selective *sharing* or *reuse* of knowledge across autonomously developed ontologies on the one hand and accommodation of the *local points of view* or *contextuality* of knowledge on the other. Our research on modular ontologies has led to:

- (a) The development of modular variants of description logics that provide mechanisms for *semantic* importing of names (including concept, role, and nominal names) across ontology modules [Bao et al., 2006a; 2006b; 2007; 2009].
- (b) Decidability and undecidability results for modular ontology languages establishing that (a) variants of distributed description logics (DDL) that allow negated roles or cardinality restrictions in bridge rules or inverse bridge rules that connect *ALC* ontologies are undecidable.
- (c) A variant of P-DL that supports role mappings between ontology modules in ALCHIO (¬) (an extension of ALC that allows general role inclusions, inverse roles, and negated roles) is decidable [Bao et al., 2008].
- (b) The development of distributed tableau-based reasoning algorithms for P-DL [Bao, Caragea, and Honavar, 2006c; 2007b]
- (c) Tools for collaborative development of package-based partial order ontologies for applications in biomedical informatics and comparative genomics [Hughes et al., 2008].
- (d) Development of a sound and complete PSPACE tableau 27pprox.27 for the Description logic ALCK, i.e., Description Logic ALC augmented with Epistemic operators to support modeling of, and inference using, knowledge of multiple agents [Tao et al., 2012].

A long-term goal of our research on modular ontologies is to transform distributed data and knowledge base applications in the same way that the World-Wide Web has transformed the construction, sharing and use of hyperlinked documents and Wiki has transformed encyclopedia construction.

Secrecy-Preserving Inference and Query Answering (Funded in part by a grant from the National Science Foundation)

Productive interaction and collaboration among business partners, different governmental agencies (e.g., intelligence, law enforcement, public policy), or independent nations acting on matters of global concern

(e.g., counterterrorism, international finance) requires the need to share information to be balanced against the need to protect sensitive or confidential information from unintended disclosure. Our work, aimed at addressing this problem focuses on the theoretical foundations of, and algorithms and software for secrecy-preserving query answering, that is answering queries using secrets, whenever it is feasible to do so without revealing secrets. Results to date include:

- (a) A framework for secrecy-preserving query answering in the simple case of hierarchical knowledge bases under open world semantics (Bao et al., 2007).
- (b) A generalization of the secrecy-preserving query answering framework to a setting with multiple querying agents (each with a set of secrets that it is not permitted to know) that can pose queries against a knowledge base and selectively share answers received with one or more other querying agents. The framework exploits the indistinguishability of an answer that is not shared (because it is a secret) from an answer that is not entailed by the knowledge base. We showed how to use this approach in Propositional Horn and the Description Logic AL knowledge bases (Tao et al., 2015).

Work in progress is aimed at:

- The development of secrecy-preserving query answering systems for a knowledge bases of practical interest in networked information systems including hierarchical, propositional, RDF description logic (DL), and probabilistic knowledge bases.
- Examination of secrecy-preserving reasoning algorithms to settings with multiple querying agents, under various restrictions on communication among agents.

Representing and Reasoning About Qualitative Preferences (Funded in part by a grant from the NSF)

The ability to represent and reason about preferences over a set of alternatives (decisions, arguments, products, policies, etc.) is central to rational decision-making. In many real-world applications, preferences are best expressed in qualitative (as opposed to quantitative) terms. Alternatives are described in terms of a set of relevant attributes. Languages for representing preferences range from those that can express only unconditional preferences to those that can express conditional preferences, relative importance of preferences, etc. Our recent work (Santhanam et al., 2016) has led to:

- (a) The first practical solution to the problem of determining whether one outcome dominates another with respect to a given set of qualitative preferences over the attributes of the outcomes (Santhanam et al., 2010). The proposed solution reduces the problem of dominance testing, to reachability analysis in a graph of outcomes. We provide an encoding of TCP-nets in the form of a Kripke structure for Computational Tree Logic (CTL). We show how to test dominance using a model checker for CTL.
- (b) Specification of dominance relation that allows comparison of collections of objects in terms of preferences over attributes of the objects that make up the collection the set of most preferred collections, and algorithms for dominance testing that are guaranteed to return only (sound), all (complete), or at least one (weakly complete) of the most preferred collections (Santhanam et al., 2011).
- (c) Applications of preference reasoning algorithms in service composition and substitution based on qualitative preferences over non-functional attributes of the services (Santhanam et al., 2008, 2009), and in minimizing credential disclosure based on qualitative preferences over sensitivity attributes of the credentials (Oster et al., 2013).

Work in progress is focused on:

- Extensions of the framework to handle reasoning with the preferences of multiple stakeholders.
- Applications of preference reasoning in product design, cyber-defense, and healthcare.

Algorithms and Software for Interactive Discovery and Composition of Web Services (Funded in part by a grant from the National Science Foundation).

Practical applications in a variety of domains, e.g., e-commerce, e-science, etc. increasingly rely on complex services that are composed from physically distributed and autonomously developed component services. Our recent work has focused on interactive methods for service composition with provable guarantees with respect to user-specified functional and non-functional requirements. Some results of this research include:

- (a) Algorithms for interactive specification-driven functional assembly of composite services from a repository of available component services (Pathak et al., 2007a; 2007b; 2008)
- (b) Algorithms for efficient identification of feasible replacement of one or more component services of a composite service while maintaining its functionality (Pathak et al., 2007)
- (c) Algorithms for incorporating user preferences over non-functional attributes of a service (e.g., cost, security, reliability) in assembling a most preferred composition that achieves the user-specified functionality (Santhanam et al., 2008).

Macromolecular Sequence-Structure-Function-Interaction- Expression Relationships (funded in part by an NIH grant 5R21GM066387 and an NSF grant)

Protein-protein, protein-DNA, and protein-RNA interactions play a pivotal role in virtually all biological processes. Reliably pinpointing which specific amino acid residues form the interface(s) between a protein and its binding partner(s) is critical for understanding the structural and physicochemical determinants of such interactions and has wide applications in modeling and validating interactions predicted by high-throughput methods, in engineering proteins, and in prioritizing drug targets. Because experimental determination of protein-protein and protein nucleic acid complexes is expensive, laborious, and error-prone, there is a need for development of reliable computational methods for identifying protein-protein interface residues. Protein and its binding partner(s) are critical for understanding the structural and physicochemical determinants of such interactions and has wide applications predicted by high-throughput methods, in engineering protein and its binding partner(s) are critical for understanding the structural and physicochemical determinants of such interactions and has wide applications in modeling and validating interactions predicted by high-throughput methods, in engineering proteins, and in prioritizing drug targets. Because experimental determination of protein-protein and protein nucleic acid complexes is expensive, laborious, and error-prone, there is a need for development of reliable computational methods for identifying protein nucleic acid complexes is expensive, laborious, and error-prone, there is a need for development of reliable computational methods for identifying protein-protein interface residues.

Against this background, our work aims to develop and systematically evaluate computational methods for computational characterization and prediction of protein-protein, protein-DNA, and protein-RNA interactions, interfaces, and complexes as well as residues and other functionally important sites (e.g., B-cell and T-cell epitopes, glycosylation, and phosphorylation sites). Some of the results to date include:

- (a) Comprehensive Database of Protein-protein Interfaces (Jordan et al., 2012) and of Protein-RNA Interfaces (Lewis et al., 2010).
- (b) Development of a state-of-the-art approach to predicting protein-RNA interface residues in protein sequences (Walia et al., 2012, Terribilini et al., 2006, 2007; El-Manzalawy et al., 2016; 2019)
- (c) Development of machine learning approaches and online servers for the prediction of protein- protein interface residues from amino acid sequence and when available, structural information (Yan et al., 2004; Towfic et al., 2011) including a state-of-the-art structure-based interface predictor (Jordan et al., 2012).
- (d) Development of sequence homology-based methods and online servers for protein interface prediction (Xue et al., 2011), including non-partner-specific methods for predicting obligate interfaces and interfaces of disordered proteins and partner-specific methods for predicting transient interfaces.
- (e) Development of sequence-based machine learning methods for predicting the approximate number of putative interaction partners of a protein (Andorf et al., 2013).

- (f) Development of a novel approach and online server for scoring docked protein-protein complex conformations using predicted partner-specific protein-protein interfaces (Xue et al., 2011; 2013; 2016; 2020).
- (g) Demonstration of the pitfalls of commonly used windows-based cross-validation for sequence- based classification tasks (e.g., phosphorylation site prediction, DNA-binding site prediction) (Caragea et al., 2009).
- (h) Application of classifiers trained using machine learning to discover a large set of incorrect Gene Ontology annotations an experimentally well-studied family of proteins mouse kinases (Andorf et al., 2007).
- (i) Development of machine learning approaches and online servers for prediction of protein-DNA interface residues from amino acid sequence, and when available, structural information (Yan et al., 2006).
- (j) Structural characterization of protein-protein and protein-RNA interfaces (Towfic et al., 2011).
- (k) Development of machine learning methods and online servers for identification of posttranslational modification sites e.g., phosphorylation sites, glycosylation sites in amino-acid sequences (Caragea et al., 2007).
- Development of machine learning methods and online servers for predicting linear and B-cell epitopes from amino acid sequences (EI-Manzalawy et al., 2008) including methods for predicting variable length and conformational B-cell epitopes.
- (m) Demonstrations of the pitfalls of commonly used benchmark datasets for evaluating the performance of machine learning approaches to MHC-II binding site prediction (El-Manzalawy, 2008).
- (n) Prediction of the designability of binary (H-P) protein sequences (Peto et al., 2008).
- (o) Prediction of protein and RNA binding sites in recalcitrant (in support of attempts at structure determination) proteins e.g., HIV-1 and EIAV and experimental confirmation of the predictions (with Lee et al., 2008).
- (p) Characterization and prediction of RiboSNitches

The online web servers can be found at <u>http://ailab.ist.psu.edu/software.html</u>.

Comparative Analysis of Biomolecular Networks (funded in part by a grant from the USDA and in part by a National Science Foundation IGERT fellowship)

Network models play an increasingly important role in the interpretation of complex interactions among genes, proteins, regulatory RNAs, small ligands and other signaling agents. Comparative analysis of network models of biomolecular interactions across different species or tissues has emerged as an important tool for identifying conserved modules, predicting functions of specific genes or proteins, and studying the evolution of biological processes, among other applications. Hence, there is need for scalable modular, and extensible algorithms software for construction, querying, and comparative analysis of diverse types of biomolecular networks. Our work has led to:

- (a) Development of a suite of modular graph kernel based scalable and customizable algorithms and their open-source implementations for aligning protein-protein interaction networks and gene coexpression networks (Towfic et al., 2009). Graph kernels allow efficient computation of global alignment of networks by decomposing the task into a set of local graph kernel computations. The resulting software is available at http://ailab1.ist.psu.edu/BinaWebApp/.
- (b) Application of comparative protein-protein interaction network analyses to reliably distinguish orthologs from paralogs (Towfic et al., 2010) and of comparative gene co-expression network analyses to identify B-cell ligand processing pathways (Towfic et al., 2012).

- (c) Characterization of gene expression changes during the onset of photosynthesis (Lonosky et al., 2004), differentiation of retinal stem cells into rod photoreceptors (Hecker et al., 2010).
- (d) Characterization differences in the proteome of murine retinal and brain derived progenitor cells (Dunn-Thomas et al., 2008).
- (e) Development of databases and software tools for capture, analysis, annotation, and integration of gene expression data with other types of 'omics' data (Couture et al., 2009).
- (f) Development of BioNetwork Bench, an open source, user-friendly suite of database and software tools for constructing, querying, and analyzing gene and protein network models (Kohutyuk et al., 2012; Hecker et al., 2008).
- (g) Development and analysis of a machine learning algorithms for inference of temporal Boolean network models from multivariate time series data, with applications to inference of genetic networks from gene expression data (Silvescu and Honavar, 2001).

Work in progress is aimed at the:

- Further development of BiNA, our modular, extensible, and scalable suite of graph kernel based algorithms to enable alignment of richer networks including (a) Undirected graphs that contain multiple types of links (e.g., interaction, co-localization, etc. in the case of protein-protein interaction networks), or multiple types of nodes (e.g., in the case of macromolecular interaction networks that simultaneously model the interactions among proteins, RNA, DNA, etc.), or both; (b) Directed graphs with one or more types of links (up or down regulation of one gene by another in the case of transcriptional networks), or one or more types of nodes, or both as in the case of richly annotated signaling networks and metabolic networks; (c) The weighted counterparts of undirected (e.g., gene expression correlation networks) as well as directed graphs and (d) Undirected or directed multigraphs with multiple links between nodes as well as variants that accommodate sets of labels on nodes (e.g., Gene ontology functional annotation, subcellular localization, etc.) and links, as well as their weighted counterparts.
- Systematic evaluation of the graph kernel based network alignment algorithms (including comparisons them with existing algorithms) on several representative applications including: identifying differences in patterns of biomolecular interactions across different species or tissues; identifying conserved modules or subnetworks; predicting functions of specific genes or proteins (and identification of functional orthologs); compensating for limited experimental data concerning biomolecular interactions within one species through transfer of information from another species on several benchmark datasets.

Deciphering Brain Structure, Activity, and Function Relationships

The advent of new ways to determine brain structure and measure brain activity offer unprecedented opportunities to understand the complex relationship between how brains perform cognition and orchestrate behavior in naturalistic settings. Against this background, our work is aimed at developing and applying novel computational methods for:

- Understanding functional brain connectivity from brain activity (e.g., fMRI) and other data.
- Comparing brain networks across individuals, tasks, or conditions
- Characterizing and modeling longitudinal changes in brain networks due to development, learning, aging, and disease.

Biologically Inspired Algorithms for Knowledge Representation, Memory, Language Processing and Learning (Funded in part by a grant from the National Science Foundation) Artificial neural networks, because of their potential for massive parallelism and fault and noise tolerance, offer an attractive approach to the design of associative memories, language processors, and trainable

pattern classifiers. Constructive learning algorithms, which build arbitrarily complex decision boundaries

needed for pattern classification (and in some ways, foreshadowed the recent development of support vector machines) were motivated by: the need to overcome the limitations of learning through parameter modification within an a priori fixed network topology; and to avoid the guesswork involved in deciding suitable network architectures for different pattern classification problems by dynamically growing the network to match the complexity of the underlying pattern classification task. Evolutionary algorithms offer a powerful means of exploring large search spaces for solutions that optimize multiple objectives e.g., feature subsets that maximize the predictive performance and minimize the complexity of the classifiers that use them. Against this background, we explored several closely related topics in biologically inspired (neural, evolutionary) algorithms and architectures for knowledge representation, language processing e.g., parsing, and learning. This work has led to:

- (a) Generalization (with convergence guarantees) of a large family of constructive neural network learning algorithms designed for 2-class binary pattern classification problems to handle classification problems involving real-valued patterns and an arbitrary number of classes (Parekh et al., 2000).
- (b) Development of a simple, inter-pattern distance based provably convergent, polynomial time constructive neural network algorithm which compares very favorably with computationally far more expensive algorithms in terms of generalization accuracy (Yang et al., 1999).
- (c) Development of algorithms for construction of robust, noise-tolerant neural memories for pattern storage and associative, content-based retrieval (Chen et al., 1995) and query processing (1996).
- (d) Development of algorithms for construction of highly parallel neural architectures for syntax analysis (parsing of regular, context-free, and context-sensitive languages) (1999).
- (e) Development of a biologically inspired neural architecture and an extended Kalman filter algorithm for place learning and localization in a-priori unknown environments which successfully accounts for a large body of behavioral and neurobiological data from animal experiments and offers several testable predictions (Balakrishnan et al., 1998, 2000).
- (f) Development of evolutionary algorithms for feature subset selection for classification problems (Yang et al., 1998) and sensors and controllers for adaptive robots (Balakrishnan and Honavar, 1996; 1998; 2001).
- (g) Development of incremental neural network learning algorithms with applications in sensing and nondestructive evaluation (Polikar et al., 2001a, 2001b, 2004).
- (h) Development of constructive neural network algorithms that take advantage of prior knowledge in the form of classification rules (Parekh et al., 1999).
- (i) Hybrid neural-symbolic architectures for information processing (Honavar and Uhr, 1994;1995).

Critical Infrastructure Monitoring and Protection (Funded in part by grants from the National Science Foundation and the US Department of Defense)

Formal methods offer a rigorous foundation for representing and reasoning about critical infrastructure for information and communication, transportation, and health. Data-driven approaches complement formal methods in domains where the available formal specifications are incomplete. Our work has used both approaches to solve problems that arise in monitoring and protecting critical infrastructure. This work has led to:

- (a) Development of model checking approaches to containing infection propagation across networks (Santhanam et al., 2011).
- (b) Development of tools for formal specification of intrusions software fault trees and of intrusion detection systems using colored Petri nets s for automated generation of multi-agent systems for coordinated intrusion detection in computer and communication networks (Helmer et al., 2002; 2006).

- (c) Development of multi-agent system for detection of coordinated or concerted attacks on distributed computing systems by monitoring different processes, resources, users, events, and extract and integrate relevant information from disparate sources over multiple space and time scales (Helmer et al., 2003Wang et al., 2006).
- (d) Development and application of machine learning approaches for learning predictive rules for anomaly and misuse detection (Kang et al., 2005, 2006).
- (e) Development of an electronic nose for detection and identification of odorants using machine learning (Polikar et al., 2001).
- (f) Development and applications of machine learning methods for non-destructive inspection of nuclear power plant pipes using ultrasound (Polikar et al., 2006).
- (g) Development of a service-oriented distributed software infrastructure for monitoring distributed power systems (Pathak et al., 2006; 2007; McCalley et al., 2007; Pham et al., 2009).
- (h) Design, analysis, and evaluation of a utility-theoretic approach to routing in communication networks that supports a flexible tradeoff between delay for a specific message and the overall network load (and hence expected delay for all routed messages) using a knowledge representation scheme that enables each node in a communication network to maintain and update a small constant-size knowledge base (independent of the network size) (Mikler et al., 1996; 1997; 1998; 2001).

PUBLICATIONS AND PRESENTATIONS

Books Authored and Edited

- 1. Santhanam, G., Basu, S., and **Honavar, V.** (2016). Representing and Reasoning About Qualitative Preferences. Synthesis Lectures in Artificial Intelligence and Machine Learning. Morgan and Claypool.
- 2. Patel, M., Honavar, V. & Balakrishnan, K. (Ed.) (2001). Advances in Evolutionary Synthesis of Intelligent Agents. Cambridge, MA: MIT Press.
- 3. Honavar, V. & Uhr, L. (1994) (Ed). Artificial Intelligence and Neural Networks: Steps Toward Principled Integration. New York, NY: Academic Press.

Influential White Papers

- 1. **Honavar, V**., Hill, M., and Yelick, K. (2016). Accelerating Science: A Computing Research Agenda. A white paper prepared for the Computing Community Consortium committee of the Computing Research Association. arXiv preprint arXiv:1604.02006.
- 2. Hager G., Bryant R., Horvitz E., Matarić M., & **Honavar V.**, (2017). Advances in Artificial Intelligence Require Progress Across all of Computer Science: http://cra.org/ccc/wp-content/uploads/sites/2/2015/01/CCC-AI-Systems-2017-FINAL.pdf
- 3. Barocas, S., Bradley, E., **Honavar, V.** and Provost, F. (2017). Big Data, Data Science, and Civil Rights A white paper prepared for the Computing Community Consortium committee of the Computing Research Association. arXiv preprint arxiv:1706.03102.
- 4. **Honavar, V.**, Yelick, K., Nahrstedt, K., Rushmeier, H., Rexford, J., Hill, Mark., Bradley, E., and Mynatt, E. (2017). Advanced Cyberinfrastructure for Science, Engineering, and Public Policy. A white paper prepared for the Computing Community Consortium committee of the Computing Research Association. arXiv preprint arXiv:1707.00599.

Refereed Journal and Conference Papers

Note: Acceptance of papers for publication in the proceedings of top Computer Science conferences is typically based on rigorous peer review. Acceptance rates are typically under 30% and conference

proceedings are published and distributed by major commercial publishers (e.g., Springer-Verlag) or professional societies (e.g., Association for Computing Machinery). Dr. Honavar's work (which includes one of the 10 most cited papers in IEEE Intelligent Systems), according to Google Scholar Data (as of October 2024), has been cited more than 19,800 times (or over 500 citations on average per year during 1990-2024) and his *h*-index² is 64, and *i*10-index is 265.

- 1. Ashtekar, N., Zhu, J., and **Honavar, V.** (2025). Class Incremental Learning from First Principles: A Review. Transactions on Machine Learning Research (TMLR) <u>https://openreview.net/forum?id=sZdtTJInUg</u>.
- 2. Rauer, E., Basu, S. and **Honavar, V.** (2025). Checking Consistency of CP-Theory Preferences in Polynomial Time: In: Proceedings of the Thirty-Ninth AAAI Conference on Artificial Intelligence (AAAI-25). In press.
- 3. Dalvi, A. and **Honavar, V.** (2025) Hyperdimensional Representation Learning for Node Classification and Link Prediction. In: Proceedings of the 18th ACM International Conference on Web Search and Data Mining. In press.
- 4. Xiao, T., Yuan, Y., Chen, Z., Li, M., Liang, S., Ren, Z., **Honavar, VG** (2025). SimPER: Simple Preference Fine-Tuning without Hyperparameters by Perplexity Optimization. In: Proceedings of the Thirteenth International Conference on Learning Representations. In press.
- 5. Zhu, H., Xiao, T., **Honavar, VG** (2025). DSPO: Direct Score Preference Optimization for Diffusion Model Alignment. In: Proceedings of the Thirteenth International Conference on Learning Representations. In press.
- 6. Xiao, T., Yuan, Y., Li, M., Chen, Z., **Honavar, VG** (2025). DIL: Direct Imitation Learning for Preference Alignment and Connections to RLHF. In: Proceedings of the Thirteenth International Conference on Learning Representations. In press.
- 7. Jacobs, R., Morgan, D., Attarian, S., Meng, J., Shen, C., Wu, Z., Xie, C.Y., Yang, J.H., Artrith, N., Blaiszik, B., Ceder, G., Choudhary, K., Csanyi, G., Cubuk, E.D., Deng, B., Drautz, R., Fu, X., Godwin, J., **Honavar, V.G**., Isayev, O., Johansson, A., Martiniani, S., Ong, S.P., Poltavsky, I., Schmidt, K.J., Takamoto, S., Thompson, A.P., Westermayr, J., and Wood, B. (2025). A practical guide to machine learning interatomic potentials – Status and future. Current Opinion in Solid State & Materials Science.
- 8. Xiao, T., Zhu, H., Zhang, Z., Guo, Z., Aggarwal, C., Wang, S., and **Honavar, V.** (2024). Efficient Contrastive Learning for Fast and Accurate Inference on Graphs. In: Proceedings of the Forty-first International Conference on Machine Learning. PMLR 235:54363-54381
- 9. Ren, W., Li, X., Chen, H., Rakesh, V., Wang, Z., Das, M. and **Honavar, V**. (2024). TabLog: Test-Time Adaptation for Tabular Data Using Logic Rules. In: Proceedings of the Forty-first International Conference on Machine Learning PMLR 235:42417-42427
- Dalvi, A., Ashtekar, N., and Honavar V. (2024). Causal Effect Estimation Using Random Hyperplane Tessellations. In: Proceedings of the 3rd Conference on Causal Learning and Reasoning. PMLR Vol. 236. pp. 688-702
- 11. Zhu, H., Xiao, T., and **Honavar, V.** (2024). 3M-Diffusion: Latent Multi-Modal Diffusion for Language-Guided Molecular Structure Generation. In: Proceedings of the first conference on language modeling (COLM 2024). In press.
- 12. Xiao, T., Yuan, Y., Zhu, H., Li, M., and **Honavar, V.** (2024). Calibrated Preference Optimization for Direct Language Model Alignment. In: Thirty-eighth Annual Conference on Neural Information Processing Systems. In press.
- 13. Xiao, T., Li, M., Yuan, Y., Zhu, H., Chao, C., and **Honavar, V.** (2024). How to Leverage Demonstration Data in Alignment for Large Language Model? A Self- Imitation Learning Perspective. In: Proceedings of the 2024 Conference on Empirical Methods in Natural Language

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- 14. Xiao, T., Cui, C., and Zhu, H., and **Honavar, V.** (2024). GeomCLIP: Contrastive Geometry-Text Pre-training for Molecules. IEEE International Conference on Bioinformatics and Biomedicine 2024 (IEEE BIBM 2024). In press.
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- 22. Honavar, V. (1994). Toward Learning Systems That Integrate Multiple Strategies and Representations. In: Artificial Intelligence and Neural Networks: Steps Toward Principled Integration. Honavar, V. & Uhr, L. (Ed). Pp. 615-644. New York: Academic Press.
- 23. Uhr, L. & Honavar, V. (1994). Artificial Intelligence and Neural Networks: Steps Toward Principled Integration. In: Artificial Intelligence and Neural Networks: Steps Toward Principled Integration. Honavar, V. & Uhr, L. (Ed). Pp. xvii-xxxii. New York: Academic Press.

Conference Proceedings Edited

1. Honavar, V. & Slutzki, G. (Ed.) (1998). Grammatical Inference Vol. 1433. Lecture Notes in Computer Science. Berlin: Springer-Verlag.

- Banzaf, W., Daida, J., Eiben, A. Garzon, M., Honavar, V., Jakiela, M., & Smith, R. (Ed.) (1999). Proceedings of the Genetic and Evolutionary Computation Conference. San Mateo, CA: Morgan Kaufmann.
- W. Langdon, E. Cantu-Paz, K. Mathias, R. Roy, D. Davis, R. Poli, K. Balakrishnan, V. Honavar, G. Rudolph, J. Wegener, L. Bull, M. Potter, A. Schultz, J. Miller, E. Burke, N. Jonoska. (2002). (Ed). Proceedings of the Genetic and Evolutionary Computing Conference. Palo Alto, CA: Morgan Kaufmann.
- H. J. Caulfield, S.-H. Chen, H.-D. Cheng, R. Duro, V. Honavar, E. E. Kerre, M. Lu, M. G. (2002). Romay, T. K. Shih, D. Ventura, P. P. Wang, and Y. Yang, editors, 2002. Proceedings 6th Joint Conference on Information Sciences, JCIS / Association for Intelligent Machinery.

Plenary Lectures, Invited Keynotes Invited Conference Talks, Distinguished Lectures

- 1. Invited Keynote Talk, Relational Causal Models, SIAM Conference on Data Mining, 2023
- 2. Invited Talk, The Promise and Potential of AI, Machine Learning and Data Science in Integrating Data and Models Across Modalities, Scales, and Model Systems, NIH Workshop on Validation of Animal Models for Biomedical Research, January 2021.
- 3. Invited Plenary Talk, On the Importance of Causal Models in Making Sense of Big Data, Workshop on Brain, Computation, and Learning, Indian Institute of Science, 2019.
- 4. Invited Plenary Talk, An excursion into Network Neuroscience, Workshop on Brain, Computation, and Learning, Indian Institute of Science, 2018.
- 5. Invited Plenary Talk, Brain Sciences Meet Big Data. Workshop on Brain, Computation, and Learning, Indian Institute of Science, 2017
- 6. Invited Plenary Talk, Foundations of Data Science: Mind the Gaps! Workshop on Transdisciplinary Foundations of Data Science. Institute for Mathematics and Applications, University of Minnesota, 2016.
- 7. Plenary Talk, Accelerating Science: A Grand Challenge for AI? AAAI/CCC Symposium on Accelerating Science: A Grand Challenge for AI. 2016.
- 8. Invited Talk, Uncertainty in AI and Machine Learning. CCC Workshop on Uncertainty in Computation. 2014.
- 9. Invited Talk, Informatics Challenges in Understanding Interactions of Food, Energy, and Water Systems, NSF INFEWS Workshop, 2015.
- 10. Invited Keynote Talk, Computational Analysis and Prediction of Protein Interfaces and Interactions. 2014 Mid-south Computational Biology and Bioinformatics Conference, 2014
- 11. Invited Keynote Talk, From Big Data Analytics to Computational Discovery and Discovery Informatics. 9th IEEE International Conference on Collaborative Computing: Networking, Applications and Worksharing, Austin, Texas, 2013.
- 12. Invited Talk, From Data Analytics to Discovery Informatics. NIH NIAID Symposium on Unlocking the Power of Big Data. National Institutes of Health, 2013.
- 13. Invited Keynote Talk, From Big Data Analytics to Discovery Informatics. Conference on Complex Adaptive Systems, Washington DC. November 2012.
- 14. Invited Talk, Computational Prediction of Protein Interfaces, and Interactions. Conference on Modeling Protein Interactions, Lawrence, Kansas, November 2012.
- 15. Invited Keynote Talk, Learning Predictive Models from Distributed Data. Conference on Intelligent Data Understanding, Boulder, CO, October 2012.
- 16. Invited Keynote Talk, Humanities as Information Sciences. Chicago Colloquium on Digital Humanities

and Computer Science, Chicago, November 2009.

- 17. Invited Keynote Talk, Aligning Macromolecular Networks. Sixth International Biotechnology and Bioinformatics Symposium (BIOT 2009), Lincoln, Nebraska, October 2009.
- 18. Invited Plenary Talk, Machine Learning in Bioinformatics, Annual Conference of the Italian Association for Artificial Intelligence (AI*IA 2008), Cagliari, Italy, September 2008.
- 19. Invited Keynote Talk, International Congress on Pervasive Computing and Management (ICPCM 2008), New Delhi, India, December 2008.
- 20. Invited Talk, Telluride Meeting on Characterizing the Landscape from Biomolecules to Cellular Networks, Telluride, Colorado, July 2008.
- 21. Invited Talk, Privacy-preserving Reasoning, Semantic Technology Conference, San Jose, CA, USA, May 2008
- 22. Invited Keynote Talk, Computational Structural Bioinformatics Workshop, IEEE Conference on Bioinformatics and Biomedicine, Silicon Valley, 2007.
- 23. Invited Talk, Making Biology and Medicine a Predictive Science. NSF Workshop on Biomedical Informatics. Oregon, 2007.
- 24. Invited Talk, Knowledge Acquisition from Semantically Disparate Distributed Data. NSF Workshop on Next Generation Data Mining and Cyber-Enabled Discovery, Baltimore, Maryland, 2007.
- 25. Invited Talk, On Selective Sharing and Reuse of Ontologies, Semantic Technology Conference, San Jose, CA, USA, May 2007
- 26. Invited Keynote Talk, Semantic Web for Collaborative e-Science, International Conference on Intelligent Sensing and Information Processing, Bangalore, India, 2006.
- 27. Invited Lecture: Querying Semantically Heterogeneous Data Sources from a User's Point of View, Semantic Technology Conference, San Jose, CA, USA, March 2006.
- 28. Invited Plenary Talk, Algorithms and Software for Collaborative Discovery from Semantically Heterogeneous, Distributed, Autonomous Information Sources Sixteenth International Conference on Algorithmic Learning Theory (ALT 2005) and Eighth International Conference on Discovery Science (DS 2005). Singapore.
- 29. Plenary Talk, Data-Driven Discovery of Macromolecular Sequence-Structure-Function Relationships. International Conference on Intelligent System Design and Applications, 2003.
- 30. Invited Talk, Agent-Based Distributed Intelligent Information Networks for Computational Inference and Knowledge Discovery in Bioinformatics. In: Workshop on Agents in Bioinformatics, Italy, 2002.
- 31. Plenary Talk, Computational Discovery of Protein Sequence-Structure-Function Relationships, Diversity in Information Science and Technology, Nebraska EPSCOR Conference, 2002
- 32. Invited Keynote Talk, Learning from Large, Distributed, Heterogeneous Data Sets. International Symposium on Artificial Intelligence (ISAI 2001), Kolhapur, India.
- 33. Invited Talk, Distributed Intelligent Information Networks. Midwestern Conference on Artificial Intelligence and Cognitive Science, 2000.
- 34. Invited Talk, Cumulative Learning in Open Environments. International Workshop on Current Computational Architectures Integrating Neural Networks and Neuroscience. Durham Castle, United Kingdom. 2000.
- 35. Invited Talk, Distributed Knowledge Networks. Artificial Intelligence for Distributed Information Networks (AiDIN '99) Workshop held during the 1999 National Conference on Artificial Intelligence (AAAI 99), Orlando, Florida. July 1999.

Juried Papers, Lightly Refereed Papers, Extended Abstracts, and Posters in Conferences and Workshops

- 1. Santhanam, G., Basu, S., and Honavar, V. (2011). Identifying Sustainable Designs Using Preferences Over Sustainability Attributes. In: AAAI Spring Symposium on Artificial Intelligence in Sustainable Design. Stanford, CA.
- 2. Caragea, C., Silvescu, A., Caragea, D. and Honavar, V. (2009). Abstraction Augmented Markov Models. In: NIPS Workshop on Machine Learning in Computational Biology (MLCB).
- 3. Tu, K., and Honavar, V. (2009). An Empirical Study of Hierarchical Dirichlet Process Priors for Grammar Induction. In: NIPS Workshop on Grammar Induction, Representation of Language, and Language Learning.
- 4. Yakhnenko, O. and Honavar, V. (2009). Multiple label prediction for image annotation with multiple kernel correlation models. In: CVPR Workshop on Visual Context Learning.
- Santhanam, G., Basu, S., and Honavar, V. (2008). On Utilizing Qualitative Preferences in Web Service Composition: A CP-net based approach 2nd International Workshop on Web Service Composition and Adaptation (WSCA) 2008
- 6. Towfic, F., Gemperline, D., Caragea, C., Wu, F., Dobbs, D., and Honavar, V. Structural Characterization of RNA-Binding Sites of Proteins: Preliminary Results. *IEEE BIBM Computational Structural Bioinformatics Workshop*, 2007.
- 7. Andorf, C., Dobbs, D., and Honavar, V. Potential Errors in Mouse Protein Gene Ontology Annotations Returned by AmiGO. Oral Presentation in: Gene Ontology Users Workshop, MGED, Seattle, Washington, September 2006.
- 8. A Bao, J., Caragea, D., and Honavar, V. (2006). A Distributed Tableau Algorithm for Package- based Description Logics. Proceedings of the Second International Workshop on Context Representation and Reasoning (CRR 2006), Riva del Garda, Italy, CEUR. 2006
- Bao. J. and Honavar, V. (2006) Divide and Conquer Semantic Web with Modular Ontologies A Brief Review of Modular Ontology Language Proposals. First International Workshop on Modular Ontologies (WoMo2006). International Semantic Web Conference, Athens, GA, 2006.
- Bao. J. and Honavar, V. (2006) Adapt OWL as a Modular Ontology Language (Position Paper). Accepted by OWL: Experiences and Directions (OWLED 2006). International Semantic Web Conference, Athens, GA. CEUR Report. Vol. 216.
- 11. Caragea, D. and Honavar, V. (2006). Knowledge Discovery from Disparate Earth Data Sources. Second NASA Data Mining Workshop: Issues and Applications in Earth Sciences. Poster Session. Pasadena, CA, May 23-24, 2006.
- Pathak, J., Basu, S., and Honavar, V. (2006). Modeling Web Service Composition Using Symbolic Transition Systems. AAAI '06 Workshop on AI-Driven Technologies for Services- Oriented Computing (AI-SOC), Boston, MA, 2006.
- J. Pathak, S. Basu, R. Lutz, and V. Honavar. (2006). MoSCoE: A Framework for Modeling Web Service Composition and Execution. IEEE Conference on Data Engineering Ph.D. Workshop, Atlanta, GA, 2006.
- Sander, J., Fu, F. Terribilini, M., Townsend, J., Winfrey, R., Wright, D., Lee, J.J., Zaback, P., F. Wu, F., Honavar, V., Voytas, D. and Dobbs, D. (2006) Designing C2H2 Zinc Finger Proteins to Target Specific Sites in Genomic DNA. 10th Annual Pacific Symposium on Biocomputing (PSB 2006), Maui, Hawaii. Poster Presentation.

- 15. Andorf, C., Dobbs, D., and Honavar, V. (2006) Learning classifiers for assigning sequences to subcellular localization families. Intelligent Systems in Molecular Biology (ISMB 2006), Fortaleza, Brazil. Poster Presentation.
- 16. EL-Manzalawy, Y., Caragea, C., Dobbs, D., Honavar, V. (2006) On the quality of motifs for protein phosphorylation site prediction. Intelligent Systems in Molecular Biology (ISMB 2006), Fortaleza, Brazil. Poster Presentation.
- 17. Terribilini, M., Sander, J., Olson, B., Lee, J.-H., Jernigan, R., Honavar, V., and Dobbs, D. (2006) A computational method to identify amino acid residues involved in protein-RNA interactions. Intelligent Systems in Molecular Biology (ISMB 2006), Fortaleza, Brazil. Poster Presentation.
- Andorf, C., Silvescu, A., Dobbs, D. and Honavar, V. (2005). Learning Classifiers for Assigning Proteins to Gene Ontology Functional Families. Poster Presentation. Intelligent Systems in Molecular Biology (ISMB 2005).
- Bao, J. and Honavar, V. (2005). Collaborative Package-Based Ontology Building and Usage. In: IEEE Workshop on Knowledge Acquisition from Knowledge Acquisition from Distributed, Autonomous, Semantically Heterogeneous Data and Knowledge Sources. Held with the IEEE International Conference on Data Mining (ICDM 2005), Houston, Tx.
- 20. Caragea, C., Caragea, D., and Honavar, V. (2005). Learning Support Vector Machine Classifiers from Distributed Data. Proceedings of the 22nd National Conference on Artificial Intelligence (AAAI 2005).
- Caragea, D., Silvescu, A., Bao, J., Pathak, J., Andorf, C., Yan, C., Dobbs, D., and Honavar, V. (2005) Poster presentation. Knowledge Acquisition from Semantically Heterogeneous, Autonomous, Distributed Data Sources. Intelligent Systems in Molecular Biology (ISMB 2005).
- 22. Terribilini, M., Yan, C., Lee, J-H, Honavar, V. and Dobbs, D. (2005). Computational Prediction of RNA binding sites in Proteins based on Amino Acid Sequence. Poster Presentation. Intelligent Systems in Molecular Biology (ISMB 2005).
- 23. Terribilini, M., Lee, J-H., Sen, T., Yan, C., Andorf, C., Sparks, W., Carpenter, S., Jernigan, R., Honavar, V., and Dobbs, D, (2005). Computational Identification of RNA binding sites in proteins. Poster presentation. Pacific Symposium on Biocomputing (PSB 2005).
- 24. Vasile, F., Silvescu, A., Kang, D-K., and Honavar, V. (2005): TRIPPER: Rule Learning Using Attribute Value Taxonomies. In: AAAI-05 Workshop on Human-Comprehensible Machine Learning.
- 25. Yan, C., Terribilini, M., Wu, F., Dobbs, D. and Honavar, V. (2005). A Computational Method for Identifying Amino Acid Residues Involved in Protein-DNA interactions. Poster Presentation. Intelligent Systems in Molecular Biology (ISMB 2005).
- Bao, J. and Honavar, V. Collaborative Ontology Building with Wiki@nt. In: Proceedings of the Third International Workshop on Evaluation of Ontology Building Tools, http://km.aifb.uni-65arlsruhe.de/ws/eon2004/EON2004_Proceedings.pdf. The Third International Semantic Web Conference (ISWC-0004), Hiroshima, 2004.
- D.-K. Kang, A. Silvescu, J. Zhang, and V. Honavar, "Generation of Attribute Value Taxonomies from Data and Their Use in Data-Driven Construction of Accurate and Compact Naive Bayes Classifiers," Proceedings of ECML/PKDD-2004 Knowledge Discovery and Ontologies Workshop (KDO-2004), Pisa, Italy, September 24, 2004.
- 28. Silvescu A., and Honavar V. (2004). A Graphical Model for Shallow Parsing Sequences. In: The AAAI-04 Workshop on Adaptive Text Extraction and Mining (ATEM-2004). July 2004, San Jose CA.
- 29. Yan, C., Honavar, V. and Dobbs, D. (2004). Application of a Two-Stage Method for Identification of

Protein-Protein Interface Residues. Poster Presentation. Eighth Annual International Conference on Research in Computational Molecular Biology (RECOMB 2004).

- 30. Caragea, D., Reinoso-Castillo, J., Silvescu, A., and Honavar, V. Statistics Gathering for Learning from Heterogeneous, Distributed, Autonomous Data Sources. In: Proceedings of the Workshop on Information Integration on the Web. International Joint Conference on Artificial Intelligence, Acapulco, Mexico, 2003.
- 31. Atramentov, A., and Honavar, V. Speeding up Multi-Relational Data Mining. In: Proceedings of the Workshop on Learning Statistical Models from Relational Data. International Joint Conference on Artificial Intelligence, Acapulco, Mexico, 2003.
- 32. Honavar, V., Dobbs, D., Jernigan, R., Caragea. D., Reinoso-Castillo, J., Silvescu, A., Pathak, J., Andorf, C., Yan, C., and Zhang, J. (2003). Algorithms and Software for Information Extraction, Integration, and Data-Driven Knowledge Acquisition from Heterogeneous, Distributed, Autonomous, Biological Information Sources. Poster Presentation. Biomedical Information Science and Technology Initiative (BISTI) Symposium; Digital Biology: The Emerging Paradigm. National Institutes of Health.
- 33. Silvescu A., and Honavar V. (2003) Ontology Elicitation: Structural Abstraction = Structuring + Abstraction + Multiple Ontologies. Poster presentation. Learning Workshop, Snowbird, Utah, 2003.
- Leiva, H., Atramentov, A., and Honavar, V. (2002). Experiments with MRDTL A Multirelational Decision Tree Learning Algorithm. In: Proceedings of the Workshop on Multi- Relational Decision Tree Learning. <u>http://www-ai.ijs.si/SasoDzeroski/MRDM2002/</u>
- *35.* Silvescu, A., Reinoso-Castillo, J., Andorf, C., Honavar, V., and Dobbs, D. (2001). Ontology- Driven Information Extraction and Knowledge Acquisition from Heterogeneous, Distributed Biological Data Sources. In: Proceedings of the IJCAI-2001 Workshop on Knowledge Discovery from Heterogeneous, Distributed, Autonomous, Dynamic Data and Knowledge Sources.
- Bhatt, R., Balakrishnan, K., and Honavar, V. (2000). Representation and Learning of Spatial Maps. In: Workshop on Machine Learning of Spatial Knowledge, International Conference on Machine Learning (ICML-2000), Stanford University.
- 37. Caragea, D., Silvescu, A., and Honavar, V. (2000). Distributed and Incremental Learning Using Extended Support Vector Machines. In: Proceedings of the 17th National Conference on Artificial Intelligence. Austin, TX.
- Caragea, D., Silvescu, A., and Honavar, V. (2000). Multi-Agent Learning from Distributed Data Sources. In: Workshop on Multi-Agent learning: Theory and Practice International Conference on Machine Learning (ICML-2000), Stanford University.
- Caragea, D., Silvescu, A., and Honavar, V. (2000). Agents that Learn from Distributed Dynamic Data Sources. In: Proceedings of the Workshop on Learning Agents, Agents 2000/ECML 2000. Stone, P. and Sen, S. (Ed.) ECML. Barcelona, Spain. Pp. 53-61.
- 40. Caragea, D., Silvescu, A., and Honavar, V. (2000). Distributed, Parallel, and Incremental Learning: A Theoretical Model. In: KDD 2000 Workshop on Distributed and Parallel Knowledge Discovery. Boston, MA.
- 41. Silvescu, A., and Honavar, V. (2000). Genetic Network Inference from Gene Expression Data. In: Workshop on Learning from Sequential and Temporal Data. International Conference on Machine Learning (ICML 2000), Stanford University.
- 42. Helmer, G., Wong, J., Honavar, V., and Miller, L. (1999). Data-Driven Induction of Compact Predictive Rules for Intrusion Detection from System Log Data. In: Proceedings of the Conference on Genetic and Evolutionary Computation (GECCO 99). San Mateo, CA: Morgan Kaufmann. Pp. 1781.

- 43. Tiyyagura, A., Chen, F., Yang, J., and Honavar, V. (1999). Feature Subset Selection in Rule Induction. In: Proceedings of the Conference on Genetic and Evolutionary Computation (GECCO 99). San Mateo, CA: Morgan Kaufmann. Pp. 1800.
- 44. Honavar, V. (1997). The Design Process: A Computational Perspective. In: Proceedings of the NSF Workshop on Decision-based Design, Sacramento, CA.
- 45. Balakrishnan, K. & Honavar, V. (1996). Experiments in Evolutionary Synthesis of Neurocontrollers. In: Proceedings of the Thirteenth National Conference on Artificial Intelligence. AAAI Press. Vol. 2. Pp. 1378.
- 46. Parekh, R. & Honavar, V. (1996). An Incremental Interactive Algorithm for Grammar Inference. In: Proceedings of the Thirteenth National Conference on Artificial Intelligence. AAAI Press. Vol. 2. Pp. 1397.
- 47. Parekh, R., Yang, J. & Honavar, V. (1996). In: Proceedings of the Thirteenth National Conference on Artificial Intelligence. AAAI Press. Vol. 2. Pp. 1398.
- 48. Honavar, V. (1993). Learning with Symbolic and Subsymbolic Representations: Some Possibilities for Vision. In: Proceedings of the AAAI Fall Symposium on Machine Learning in Computer Vision. Raleigh, North Carolina. (Also published as AAAI Tech. Rep. FS 93-04). Pp. 162-166.
- 49. Honavar, V. (1992). Generalized Distance Measures A Basis for the Integration of Symbolic and Connectionist Learning. In: Workshop on Integrating Neural and Symbolic Processes The Cognitive Dimension. AAAI-92, San Jose, California.
- 50. Honavar, V. (1992). Symbolic and Sub-symbolic Computation in Biological Neural Circuits and Systems. In: Neural Information Processing Systems Post-Conference Workshop on Symbolic and Sub-symbolic Computation in Biological Neural Circuits and Systems. Vail, Colorado.
- 51. Honavar, V. (1991). Generative Learning in Generalized Connectionist Networks. In: Constructive Induction Session Eighth International Workshop on Machine Learning. Evanston, IL.
- 52. Honavar, V. (1991). Language and Knowledge: Communication, Acquisition, and Evolution. Invited presentation in: Second International Workshop on Human and Machine Cognition. Perdido Key, Florida.
- 53. Mikler, A., Honavar, V. & Wong, J. (1992). A Knowledge-Based Approach to Dealing with Uncertain and Incomplete Information in Communication Network Management. In: Proceedings of the First Canadian Workshop on Uncertainty Management: Theory and Practice. Vancouver, B. C., Canada. Pp. 30-38.
- 54. Honavar, V. (1991). Toward Integrated Models of Natural Language Evolution, Development, Acquisition, and Communication in Multi-Agent Environments. In: Powers, D. and Reeker, L. (Ed.) Proceedings of the AAAI Spring Symposium on Machine Learning of Natural Language and Ontogeny. (MLNLO '91) pp. 82-86. Kaiserslautern, Germany: German AI Centre (DFKI).
- 55. Honavar, V. (1990). Toward Generalized Connectionist Networks: An Integration of Symbolic and Sub-Symbolic Approaches to the Design of Intelligent Systems. In: AAAI-90 Workshop on the Integration of Symbolic and Neural Processes. Boston, MA.
- 56. Honavar, V. (1990). Generative Learning Algorithms for Connectionist Networks. In: NIPS-90 Post-Conference Workshop on Constructive and Destructive Learning Algorithms. Keystone, CO.

Invited Book Reviews

1. Honavar, V. (1990). Parallel Distributed Processing: Implications for Psychology and Neurobiology. Invited review. Connection Science.

2. Honavar, V. (1992). Neural Network Design and the Complexity of Learning. Invited review. Machine Learning 9 95-98.

Theses and Dissertations

- Honavar, V. (1990). Generative Learning Structures and Processes for Generalized Connectionist Networks. Doctoral Dissertation. Madison, WI: Computer Sciences Dept. University of Wisconsin-Madison. Advisor: Professor Leonard Uhr.
- 2. Honavar, V. (1984). Automated Analysis of Dark-Field Autoradiographs. Masters Thesis. Philadelphia, PA: Center for Image Processing and Pattern Recognition. Department of Electrical and Computer Engineering. Drexel University. Advisor: Professor Oleh Tretiak.

Selected Plenary or Invited Talks

- 1. Plenary Talk, Relational Causal Models, SIAM Conference on Data Mining. 2023
- 2. **Keynote Talk,** On the importance of causal models in making sense of big data, US-Serbia and West Balkan Workshop on Data Science, Belgrade, Serbia. 2018
- 3. **Plenary Talk,** Data Science Meets Brain Science, Workshop on Brain, Computation, and Learning, Indian Institute of Science, 2018.
- 4. **Plenary Talk,** Transdisciplinary Foundations of Data Science. Workshop on Brain, Computation, and Learning, Indian Institute of Science, 2017.
- 5. **Plenary Talk,** Data Analytics, and the Internet of Things. U of Albany President's Forum on Data. 2017.
- 6. **Plenary Talk,** Transdisciplinary Foundations of Data Science: Mind the Gaps. Institute for Mathematics and Its applications, University of Minnesota, 2016.
- 7. **Invited Lecture**, From Data Analytics to Computational Discovery and Discovery Informatics, Arizona State University. 2013.
- 8. **Bortree Lecture,** Computational Prediction of Protein Interfaces and Interactions, Pennsylvania State University. 2013.
- 9. **Distinguished Lecture**, Computational Prediction of Protein Interfaces and Interactions, Georgia State University. January 2013.
- 10. **Distinguished Lecture**, From Big Data Analytics to Discovery Informatics. Pennsylvania State University, December 2012.
- 11. **Invited Colloquium,** Computational Prediction of Protein Interfaces and Interactions, University of California Irvine, September 2012.
- 12. **Invited Colloquium,** Computational Prediction of Protein Interfaces, and Interactions. University of North Texas, June 2012.
- 13. **Invited Talk,** Towards Infrastructure for Collaborative Discovery. IciS Workshop on Integrating, Representing, and Reasoning over Human Knowledge, August 2010.
- 14. **Invited Talk**, Knowledge Acquisition from Semantically Disparate, Distributed Data. CISE (IIS), National Science Foundation, May 2010.
- 15. **Invited Lecture**, From Annotating Sequences to Aligning Networks. Computation in Biology and Medicine Annual Retreat, University of Wisconsin-Madison, October 2009.
- 16. **Invited Colloquium,** Transforming Biology from a Descriptive Science into a Predictive Science, Indian Institute of Information Technology, Bangalore, India, January 2009.

- 17. **Invited Colloquium,** Transforming Biology from a Descriptive Science into a Predictive Science: Predictive Models of Macromolecular Function and Interaction. Bioinformatics Center, University of Pune, India, December 2008.
- Invited Colloquium, Semantics-Enabled Infrastructure for Collaborative, Integrative e- Science. School of Information Technology, Jawaharlal Nehru University, New Delhi, India, December 2008.
- 19. **Invited Talk,** Computational Sciences. High Performance Computing Center, Jawaharlal Nehru University, New Delhi, India, December 2008.
- 20. **Invited Colloquium,** Semantics-enabled infrastructure for collaborative, integrative e-science. Yahoo!, Bangalore, India, January 2008.
- 21. **Invited Colloquium,** Algorithms and Software for Knowledge Acquisition from Semantically Heterogeneous, Distributed Data Sources. Dept. of Electrical and Computer Engineering. University of Iowa. 2006.
- 22. **Invited Colloquium,** Algorithms and Software for Collaborative Discovery in Systems Biology. Dept. Biostatistics, Bioinformatics & Epidemiology. Medical University of South Carolina, 2006.
- 23. **Invited Talk,** Algorithms and Software for Knowledge Acquisition from Semantically Heterogeneous, Distributed, Autonomous Information Sources. Google Research, 2005.
- 24. **Invited Talk,** All Science is Computer Science. Iowa Undergraduate Consortium. Drake University, 2004.
- 25. **Invited Colloquium,** Computational Discovery of Protein Sequence-Structure-Function Relationships: Bioinformatics Infrastructure and Sample Applications. University of Wisconsin-Madison Biostatics and Medical Informatics Department. 2002.
- 26. **Invited Talk,** Algorithmic and Systems Approaches to Computer Assisted Knowledge Discovery from Biological Data. Iowa State University University of Iowa Joint Workshop on Bioinformatics. November 3-4, 2000.
- 27. **Invited Talk,** Neuromimetic Adaptive Autonomous Intelligent Systems. Institute for Computer Applications in Science and Engineering. NASA-Langley Research Center. Hampton, VA. September 28, 1999.
- 28. **Invited** Colloquium, Kolmogorov Complexity and Computational Learning Theory: Some Emerging Connections and Recent Results. Center for Neural Basis of Cognition, Carnegie Mellon University and University of Pittsburgh, Pittsburgh, PA. 1998.
- 29. **Invited Colloquium,** Experiments in Evolutionary Robotics. Department of Mathematics and Computer Science, Grinnell College, Iowa. October 1996.
- 30. **Invited Lecture,** Data Mining and Knowledge Discovery. Irish Life, Des Moines, Iowa. September 1996.
- 31. **Invited Lecture,** Knowledge Acquisition through Machine Learning. Principal Mutual, Des Moines, Iowa. January 1994.
- 32. **Invited Colloquium,** Generalized Connectionist Networks and Processes for Intelligent Systems. International Computer Science Institute, Berkeley, *CA.* (1990).
- 33. **Invited Colloquium,** Generative Learning Structures and Processes for Generalized Connectionist Networks. Cognitive and Learning Systems Laboratory, Siemens Research, Princeton, NJ. (1990).

Invited Tutorials

- 1. Honavar, V. Tutorial: Semantics-Enabled e-Science Cyberinfrastructure for Data Mining, 15th Italian Symposium on Advanced Database Systems. Torre Canne, Italy.
- Honavar, V. Tutorial: Machine Learning Approaches in Computational and Systems Biology. International Conference on Intelligent Sensing and Information Processing, Bangalore, India, 2006
- 3. Honavar, V. and Caragea, D. Tutorial: Semantic Web for Collaborative Knowledge Acquisition, IEEE International Conference on Digital Information Management, Bangalore, India, 2006.
- 4. Honavar, V. and Caragea, D. Tutorial: Collaborative Knowledge Acquisition from Semantically Disparate, Distributed Data Sources, 2006 International Symposium on Collaborative Technologies and Systems, Las Vegas, Nevada, USA, May 2006.
- 5. Honavar, V. and Caragea, D. Semantic Web Technologies for Collaborative Knowledge Acquisition, International Conference on Digital Information Management, Bangalore, India, December 2006.
- 6. Honavar, V. Intelligent Agents and Multi-Agent Systems IEEE Conference on Evolutionary Computation (CEC), Washington, DC. 1999.
- 7. Honavar, V. Computational Learning Theory, Genetic Programming Conference, Stanford, 1997.
- 8. Honavar, V. Intelligent Agents, Genetic Programming Conference, Madison, WI, 1998.

Invited Panel Presentations

- 1. Panel on Data Science Training for Social and Behavioral Sciences, National Institutes of Health, 2017.
- 2. Panel on Career Pathways for PhDs in AI and Related Areas. SIGAI Career Network and Conference, Boston, MA 2016.
- 3. Panel on Big Data, Dupont Summit, Washington DC, 2013.
- 4. Panel on Big Data Research Opportunities, IEEE International Conference on Big Data, 2013.
- 5. Panel on Big Data and Discovery Informatics, AAAI Fall Symposium on Discovery Informatics, Washington DC, November 2012.
- 6. Panel on Big Data Research Opportunities and Challenges in Biological Sciences, ACM Conference on Bioinformatics and Computational Biology, Orlando, Florida, 2012.
- 7. Panel on Digital Humanities and Computer Science, Chicago Colloquium on Digital Humanities and Computer Science, Chicago, November 2009.
- 8. Panel on Data Mining Careers, SIAM Conference on Data Mining (SDM 2009), April 2009.
- 9. Panel on Interdisciplinary Research and Training in Bioinformatics and Computational Biology, Annual Conference of the Italian Association for Artificial Intelligence (AI*IA 2008), Cagliari, Italy, September 2008.
- 10. Panel on Semantic Data Integration. NSF Workshop on Biomedical Informatics, 2007.
- 11. Panel on Learning in Knowledge-Based Systems. Second World Congress on Expert Systems. Lisbon, Portugal (1994).
- 12. Panel on Hybrid Architectures for Intelligent Systems. Second World Congress on Expert Systems. Lisbon, Portugal (1994).
- 13. Panel on Hybrid Intelligent Systems (SIGHI meeting) World Congress on Neural Networks. San Diego, U.S.A. (1994).

SOFTWARE, DATABASES, SERVERS

- INDUS: Algorithms and Software for Learning Predictive Models from Distributed Data:
 - Indus Learning Framework
 - Indus Integration Framework
- iPref-R: A Qualitative Preference Reasoner.
- Biomolecular Network Alignment Toolkit.
- Bionetworkbench.
- Database of Protein-protein Interfaces.
- Gennotate: A Genome Annotation Toolkit.
- NPS-HomPPI: Non-Partner-Specific Sequence Homology-Based Protein-Protein Interface Prediction Server.
- PS-HomPPI: Partner-Specific Sequence Homology Based Protein-Protein Interface Prediction Server.
- PrISE: A Local Structural Similarity Based Protein-Protein Interface Prediction Server.
- Dock Rank: Ranking Docked Models Based on Predicted Interfaces.
- ANExDB: Animal Gene Expression Database.
- Protein-RNA Interface Prediction Server.
- MHC-II Binding Affinity Prediction Server.
- B-cell epitope Prediction Server.
- Epitope Prediction Toolkit.

STUDENT MENTORING

I find working with graduate and undergraduate students to be an extremely rewarding experience. I work with exceptional Ph.D. students with diverse backgrounds – ranging from very theoretical to very experimental. I also enjoy working with M.S. students and undergraduates interested in research. My students benefit from strong mentoring and close interactions within a very collaborative research group. Research-based training in my research group emphasizes development of skills and expertise necessary for the pursuit of a successful independent research career:

- (a) Ability to identify and formulate fundamental research problems.
- (b) Ability to critically review scientific work.
- (c) Ability to conceive, plan, and propose research projects.
- (d) Ability to develop creative and innovative solutions.
- (e) Strong experimental and/or theoretical expertise in relevant areas.
- (f) Effective writing and presentation skills.
- (g) Ability to develop and sustain productive research collaborations.
- (h) Strong sense of ethics and responsibility in conduct of research.

Fundamental scientific questions (e.g., what is the algorithmic basis of cumulative multi-task learning? How is information encoded, stored, retrieved, decoded, and used in biological systems? How can we precisely characterize the syntax and semantics of the language of macromolecular sequences?); or important practical problems (how do we extract, assimilate, and use information from heterogeneous, distributed, autonomous data and knowledge sources to facilitate collaborative scientific discovery in biology?) drive our research.

My group takes a problem-centered approach to research. In addition to all the usual requirements for successful research, this requires a willingness to acquire, adapt, develop, and apply techniques and tools from areas that lie outside the traditional boundaries of the discipline (e.g., Computer Science) or a sub-discipline (e.g., Machine Learning) when necessary to solve a research problem.

Graduate students who join my lab typically have a broad-based training in Computer Science or a closely related discipline. Many have a strong interest in developing algorithmic or computational models of intelligent behavior (including learning and multi-agent interaction). Some have an interest in developing and applying algorithmic tools for scientific discovery in computational biology and bioinformatics. Some have an interest in building scalable, flexible, extensible, robust, and open-ended distributed information systems. I encourage and nurture interaction among members of my group through research seminars and collaborative research projects.

All my former Ph.D. students have taken up academic careers or research-oriented careers in the industry. M.S. graduates typically end up in industry. Undergraduates who have worked in my lab often pursue graduate study at one of the other universities with strong programs in Artificial Intelligence or a related area (e.g., Computational Biology).

GRADUATE STUDENT AND POSTDOCTORAL RESEARCH SUPERVISION

Postdoctoral Fellows (Past)

- 1. **Donna Coffman** (2015-2016). Supported by an NIH K-award. Current position: Assistant Professor. Temple University.
- Ganesh Ram Santhanam (2011-2013), Research Associate, Center for Computational Intelligence, Learning, and Discovery, Iowa State University. Topics: Representing and reasoning about preferences. Model checking approaches to finding and reasoning about intervention policies in networks. Current Position: Postdoctoral Research Associate, Computer Science, Iowa State University.
- 3. **Jia Tao** (2013) Research Associate, Center for Computational Intelligence, Learning, and Discovery. Iowa State University. Topics: Epistemic Description Logics, Secrecy-preserving Query Answering. Current Position: Visiting Assistant Professor, Bryn Mawr College, Pennsylvania.
- 4. **Yasser El-Manzalawy (2010-2011).** Research Associate, Center for Computational Intelligence, Learning, and Discovery (CCILD), Iowa State University and Center for Big Data Analytics and Discovery Informatics (Pennsylvania State University). Topic: Machine learning approaches in Immune Informatics. And College of Information Sciences and Technology, Pennsylvania State University. Topic: Machine Learning and Biomedical Big Data Analytics. Yasser was supported in part by a Clinical and Translational Sciences Institute award from the National Institutes of Health.
- 5. Li Xue (2012-2013) Research Associate, Center for Computational Intelligence, Learning, and Discovery (CCILD), Iowa State University. Topic: Computational Prediction of Protein-Protein and Protein-RNA Interfaces and Interactions. Li was supported by CCILD.
- 6. **Cornelia Caragea** (2010) Research Associate, Center for Computational Intelligence, Learning, and Discovery (CCILD), Iowa State University. Topic: Machine Learning in Computational Biology.

Cornelia was supported in part on a grant from the NSF and in part by CCILD. Current position: Research Associate, Pennsylvania State University.

- 7. **George Voutsadakis,** Research Associate, Center for Computational Intelligence, Learning, and Discovery (CCILD), Iowa State University. Topics: Federated Knowledge Bases, Semantic Web, Secrecy-Preserving Reasoning. George was supported in part by the ISU NSF Industry-University Cooperative Research Center in Computer and Network Security and in part by CCILD. Current position: Associate Professor of Mathematics and Computer Science, Lake Superior State University.
- 8. **Jae-Hyung Lee** (2008-2009). Research Associate, Center for Computational Intelligence, Learning, and Discovery (CCILD), Iowa State University. Topic: Construction and Analysis of Macromolecular Interaction Networks. Jae-Hyung was supported in part by CCILD. Current Position: Research Associate, UCLA.
- 9. **Jie Bao** (2007-2008). Research Associate, Center for Computational Intelligence, Learning, and Discovery (CCILD), Iowa State University. Topic: Representing and Reasoning with Federated Ontologies: Selective Knowledge Reuse, Privacy-preserving reasoning. Jie was supported in part by a grant from the National Science Foundation and in part by CCILD. Current Position: Research Associate (with Jim Hendler), RPI.
- Doina Caragea (2004-2006) Research Associate, Center for Computational Intelligence, Learning, and Discovery (CCILD), Iowa State University. Topic: Knowledge Acquisition from Semantically Heterogeneous, Distributed Information Sources. 2004-2006. Doina is supported in part by a grant from the National Institutes of Health and in part by CCILD. Current Position: Assistant Professor of Computer Science, Kansas State University.
- 11. **Byron Olson** (2005-2006). Research Associate, Center for Computational Intelligence, Learning, and Discovery (CCILD), Iowa State University. Topic: Discovery of Macromolecular Sequence-Structure-Function Relationships, Transcriptomics, Proteomics, and Interactomics. Byron was supported in part by a grant from the National Institutes of Health and in part by CCILD. Current Position: Research Assistant Professor of Electrical and Computer Engineering, Arizona State University.

Postdoctoral Fellows (Past)

- 12. **Donna Coffman** (2015-2016). Supported by an NIH K-award. Current position: Assistant Professor. Temple University.
- 1. **Ganesh Ram Santhanam** (2011-2013), Research Associate, Center for Computational Intelligence, Learning, and Discovery, Iowa State University. Topics: Representing and reasoning about preferences. Model checking approaches to finding and reasoning about intervention policies in networks. Current Position: Current Position: Associate Scientist, Iowa State University.
- Jia Tao (2013) Research Associate, Center for Computational Intelligence, Learning, and Discovery. Iowa State University. Topics: Epistemic Description Logics, Secrecy-preserving Query Answering. Initial Position: Visiting Assistant Professor, Bryn Mawr College, Pennsylvania. Current Position: Associate Professor of Computer Science, Lafayette College, Pennsylvania.
- 2. Yasser El-Manzalawy (2010-2011). Research Associate, Center for Computational Intelligence, Learning, and Discovery (CCILD), Iowa State University and Center for Big Data Analytics and Discovery Informatics (Pennsylvania State University). Topic: Machine learning approaches in Immune Informatics. College of Information Sciences and Technology, Pennsylvania State University. Topic: Machine Learning and Biomedical Big Data Analytics. Yasser was supported in part by a Clinical and Translational Sciences Institute award from the National Institutes of Health. Current Position: Assistant Professor, Geisinger.

- 3. Li Xue (2012-2013) Research Associate, Center for Computational Intelligence, Learning, and Discovery (CCILD), Iowa State University. Topic: Computational Prediction of Protein-Protein and Protein-RNA Interfaces and Interactions. Li was supported by the Iowa State University Center for Computational Intelligence, Learning, and Discovery. Initial Employment: Postdoctoral Research Associate, Iowa State University. Current Employment: Assistant Professor of Bioinformatics, Radboud University.
- 4. Cornelia Caragea (2010) Research Associate, Center for Computational Intelligence, Learning, and Discovery (CCILD), Iowa State University. Topic: Machine Learning in Computational Biology. Cornelia was supported in part on a grant from the NSF and in part by CCILD. Initial Position: Postdoctoral Research Associate, Center for Computational Intelligence, Learning, and Discovery, Iowa State University. Current Position: Professor of Computer Science, University of Illinois at Chicago.
- 14. **George Voutsadakis,** Research Associate, Center for Computational Intelligence, Learning, and Discovery (CCILD), Iowa State University. Topics: Federated Knowledge Bases, Semantic Web, Secrecy-Preserving Reasoning. George was supported in part by the ISU NSF Industry-University Cooperative Research Center in Computer and Network Security and in part by CCILD. Current position: Associate Professor of Mathematics and Computer Science, Lake Superior State University.
- 15. **Jae-Hyung Lee** (2008-2009). Research Associate, Center for Computational Intelligence, Learning, and Discovery (CCILD), Iowa State University. Topic: Construction and Analysis of Macromolecular Interaction Networks. Jae-Hyung was supported in part by CCILD. Initial Position: Research Associate, UCLA. Current Position: Professor of Microbiology, Kyung Hee University.
- 16. **Jie Bao** (2007-2008). Research Associate, Center for Computational Intelligence, Learning, and Discovery (CCILD), Iowa State University. Topic: Representing and Reasoning with Federated Ontologies: Selective Knowledge Reuse, Privacy-preserving reasoning. Jie was supported in part by a grant from the National Science Foundation and in part by CCILD. Initial Position: Research Associate (with Jim Hendler), RPI. Current Position: CEO and Founder, Memect.
- 17. **Doina Caragea** (2004-2006) Research Associate, Center for Computational Intelligence, Learning, and Discovery (CCILD), Iowa State University. Topic: Knowledge Acquisition from Semantically Heterogeneous, Distributed Information Sources. 2004-2006. Doina is supported in part by a grant from the National Institutes of Health and in part by CCILD. Initial Position: Assistant Professor of Computer Science, Kansas State University. Current Position: Professor of Computer Science, Kansas State University.
- 18. **Byron Olson** (2005-2006). Research Associate, Center for Computational Intelligence, Learning, and Discovery (CCILD), Iowa State University. Topic: Discovery of Macromolecular Sequence-Structure-Function Relationships, Transcriptomics, Proteomics, and Interactomics. Byron was supported in part by a grant from the National Institutes of Health and in part by CCILD. Initial Position: Research Assistant Professor of Electrical and Computer Engineering, Arizona State University.

Post-Doctoral Fellows (Current)

1. **Justin Petucci.** Research Associate, Institute for Computational and Data Sciences. Topic: Predictive and causal modeling of health risks and health outcomes from electronic health records and other data sources.

Ph.D. Graduates

1. Junjie Liang (Informatics, Pennsylvania State University). 2022. Predictive modeling for high-

dimensional longitudinal data. Junjie was supported by a research assistantship funded by the National Science Foundation. Initial Employment: Research Scientist, Bloomberg AI.

- 2. **Aria Khademi** (Informatics, Pennsylvania State University). 2021. Excursions in Causal Data Science: Fairness, Causal Attribution, and Applications. Aria is supported by a research assistantship funded by the Edward Frymoyer Endowed Professorship (held by Vasant Honavar) and in part by a research assistantship funded by the National Science Foundation. Initial Employment: Research Scientist, Ford Research.
- 3. **Tsung-Yu Hsieh** (Computer Science and Engineering, Pennsylvania State University). 2021. Explainable Predictive Modeling and Causal Effect Estimation from Complex Time-varying Data. Tsung-Yu was supported by a research assistantship funded by the National Science Foundation. Initial Employment: Research Scientist, Microsoft.
- 4. **Yiwei Sun** (Computer Science and Engineering, Pennsylvania State University). 2021. Adversarial Attacks and Representation Learning for Graph-Structured Data. Yiwei was supported by research assistantships funded by the National Science Foundation and Samsung Research. Initial Employment: Research Scientist, Coupang.
- 5. **Sam Gur** (Neuroscience, Pennsylvania State University); 2019. Machine-learning-based functional connectivity analyses. Graduation: 2019. Sam was funded in part by a teaching assistantship and in part by a research assistantship supported by the Edward Frymoyer Endowed Chair. Current Employment: IBM, Haifa, Israel.
- 6. **Sangchack Lee** (Information Sciences and Technology, Pennsylvania State University); 2019. Causal Inference from Relational Data. Sanghack is supported in part by a research assistantship funded by the National Science Foundation. Initial Employment: Columbia University. Current Employment: Assistant Professor of Computer Science, Seoul National University.
- 7. **Ngot Bui** (Information Sciences and Technology, Pennsylvania State University); 2016; Labeling Actors and Uncovering Causal Accounts of their States in Social Networks and Social Media. Ngot was supported in part by a research assistantship funded by the National Science Foundation. Current Employment: Google.
- Rasna Walia (Bioinformatics and Computational Biology; Iowa State University; With Drena Dobbs); 2014. Sequence-based prediction of RNA-protein interactions. Carson was supported in part by a research assistantship funded by the National Science Foundationand a Teaching Assistantship in Computer Science. First Employment: Research Scientist, USDA, Ames, Iowa. Current employment: Data Scientist, Corteva Agriscience.
- 9. Carson Andorf (Bioinformatics & Computational Biology; Iowa State University; with Drena Dobbs), 2013. Discovering meaning from biological sequences: focus on predicting misannotated proteins, binding patterns, and G4-quadruplex secondary structures. Carson was supported by an IGERT fellowship funded by the National Science Foundation and a research assistantship funded by the National Institutes of Health. Current employment: Senior Research Scientist, USDA, Ames, Iowa.
- 10. Harris Lin (Computer Science, Iowa State University). Learning Classifiers from Linked Data. Harris was supported in part by a research assistantship funded in part by a grant from the National Science Foundation. Initial Employment: Research Scientist, US DOE Ames Laboratory, Ames, Iowa. Current Employment: The New Zealand Institute for Plant & Food Research
- 11. Li Xue (Bioinformatics and Computational Biology, Iowa State University. With Drena Dobbs). Sequence-Homology Based Methods for Protein Interface Prediction and their Application to Ranking Docked Conformations. Graduate Research Excellence Award, Ph.D., 2012. Li was supported in part by research assistantships funded by a grant from the National Institutes of Health and in part by the Iowa State University Center for Computational Intelligence, Learning, and Discovery. Initial Employment: Postdoctoral Research Associate, Iowa State University. Current Employment: Assistant Professor of Bioinformatics, Radboud University.
- 12. Hsien-chao Chou (Bioinformatics & Computational Biology; with Volker Brendel), Local assembly

and pre-mRNA splicing analysis by high-throughput sequencing data. Ph.D., 2012. Current Employment: Senior Bioinformatics Scientist, National Cancer Institute, NIH.

- 13. **Raphael Jordan** (Computer Science, Iowa State University), Ph.D., 2012. Structure-Based Prediction of Protein-Protein Interaction Sites. Graduate Research Excellence Award. Raphael was supported in part by a research assistantship funded by a grant from the National Science Foundation and in part by a teaching assistantship in Computer Science. Current Employment: Data Mining Research Scientist, Quantcast.
- 14. **Kewei Tu** (Computer Science, Iowa State University), Ph.D., 2012. Unsupervised Learning of Probabilistic Grammars. Kewei was supported by in part by a teaching assistantship in Computer Science and in part by a research assistantship funded by a grant from the National Science Foundation. Initial Employment: Postdoctoral Research Associate, Department of Statistics and Department of Computer Science, University of California Los Angeles. Current Employment: Professor and Assistant Dean of Computer Science, Shanghai Tech.
- 15. Jia Tao (Computer Science, Iowa State University; with Giora Slutzki). Topics in Knowledge Bases: Epistemic Description Logics and Secrecy-preserving Reasoning. Ph.D., 2012. Initial Employment, Postdoctoral Research Associate, Iowa State University. Current Employment: Associate Professor of Computer Science, Lafayette College.
- 16. Fadi Towfic (Bioinformatics and Computational Biology, Iowa State University; with M. Heather West Greenlee). Ph.D., 2011. Modular Algorithms for Biomolecular Network Alignment. Fadi was supported in part by a fellowship funded by an Integrative Graduate Education and Research Training (IGERT) grant from the National Science Foundation. Initial employment: Postdoctoral Research Associate, The Broad Institute of MIT and Harvard. Current Employment: Director of Bioinformatics, Bristol Myers Squibb.
- 17. **Neeraj Koul** (Computer Science, Iowa State University). Ph.D., 2011. Learning Predictive Models from Massive, Semantically Disparate Data. Neeraj was supported in part by a research assistantship funded by a grant from the National Science Foundation. Initial Employment: Machine Learning Research Scientist, GILT Group. Current Employment: Senior Principal Scientist, AI at MITRE.
- 18. Ganesh Ram Santhanam (Computer Science, Iowa State University), Ph.D., 2010. Representing and Reasoning with Qualitative Preferences for Compositional Systems. Ganesh was supported in part by research assistantships funded by a grant from the National Science Foundation. Initial Employment: Postdoctoral Research Associate, Center for Computational Intelligence, Learning, and Discovery, Iowa State University. Current Position: Associate Scientist, Iowa State University.
- 19. **George Voutsadakis** (Computer Science, Iowa State University; with Giora Slutzki), Ph.D., 2010. Federated Description Logics for the Semantic Web. George was supported in part by research assistantships funded by a grant from the National Science Foundation. Current Position: Associate Professor of Mathematics and Computer Science, Lake Superior State University.
- 20. **Cornelia Caragea** (Computer Science, Iowa State University), Ph.D., 2009. Abstraction-Based Probabilistic Models for Sequence Classification. Cornelia was supported in part by research assistantships funded by grants from the National Science Foundation and the National Institutes of Health. Initial Position: Postdoctoral Research Associate, Center for Computational Intelligence, Learning, and Discovery, Iowa State University. Current Position: Professor of Computer Science, University of Illinois at Chicago.
- 21. **Oksana Yakhnenko** (Computer Science, Iowa State University), Ph.D., 2009. Learning from Text and Images: Probabilistic Generative and Discriminative Models for Partially Labeled Data. Oksana was supported in part by a graduate teaching assistantship in Computer Science and in part by a research assistantship funded by a grant from the National Science Foundation. Initial Position:

Postdoctoral Research Associate, INRIA, Rhone-Alpes, France. Current Position: Tech Lead Manager Google.

- 22. **Kent Vander Velden** (Bioinformatics & Computational Biology, Iowa State University; with Peter Reilly), Ph.D., 2009. Modeling, Simulation, Synthesis, and Optimization of Biochemical Networks. Kent was supported in part by a graduate fellowship funded by an NSF IGERT award and by Pioneer Hi-Bred. Initial Position: Research Scientist, Pioneer Hi-Bred. Current Position: CEO, Confluence R&D.
- 23. **Yasser El-Manzalawy** (Computer Science, Iowa State University), Ph.D., 2008. Thesis: Machine Learning Approaches to Epitope Prediction. Recipient of an Iowa State University Graduate Research Excellence Award. Yasser was supported by a fellowship from the Egyptian Government. Current Position: Assistant Professor, Geisinger.
- 24. **Michael Terribilini**, (Bioinformatics & Computational Biology, Iowa State University; with Drena Dobbs), Ph.D., 2008. Thesis: Deciphering the Protein-RNA Recognition Code. Michael was supported by a Multidisciplinary Graduate Education and Training (MGET) fellowship funded by the USDA. Current Position: Associate Professor of Biology, Elon College, North Carolina.
- 25. **Feihong Wu** (Bioinformatics & Computational Biology, Iowa State University; with Robert Jernigan), Ph.D., 2009. Thesis: Protein-Protein Interfaces: Databases, Analysis, and Prediction. Feihong was supported by research assistantships funded by the Iowa State University Graduate College and a grant from the National Institutes of Health. Initial Position: Research Scientist, Yahoo! Inc. Current Position: Software Engineer, Salesforce.
- 26. Adrian Silvescu (Computer Science, Iowa State University), Ph.D., 2008; Thesis: Inductive Learning Via Abstraction and Superstructuring. Adrian was supported through a teaching assistantship from the Department of Computer Science and research assistantships funded by Pioneer Hi-Bred and the National Science Foundation. Initial Position: Research Scientist, Yahoo! Inc. Current Position: Senior Research Scientist, Naviance.
- 27.LaRon Hughes (Bioinformatics and Computational Biology, Iowa State University; with James Reecy). Ph.D., 2008. Thesis: Design, Implementation, and Some Applications of an Animal Trait Ontology. LaRon was supported in part by an NSF Integrative Graduate Education and Research Training (IGERT) Fellowship in Bioinformatics and Computational Biology. Initial Employment: Research Scientist, Genome Quest.
- 28. **Jie Bao** (Computer Science, Iowa State University). Ph.D., 2007. Thesis: Representing and Reasoning with Modular Ontologies. Jie Bao was supported by a research assistantship in Computer Science funded in part by the National Science Foundation, the Iowa State University Center for Integrative Animal Genomics, and the Center for Computational Intelligence, Learning, and Discovery. Initial Position: Research Associate, Computer Science, Rensselaer Polytechnic Institute. Current Position: CEO, Memect.
- 29. Tyra Dunn (Bioinformatics and Computational Biology, Iowa State University; with M. Heather West Greenlee). Ph.D., 2007. Thesis: Characterizing and Influencing Differentiation of Retinal Progenitor Cells. Tyra was supported in part by an Integrative Graduate Education and Research Training (IGERT) fellowship from the National Science Foundation.
- 30. **Jyotishman Pathak** (Computer Science, Iowa State University). Ph.D., 2007. Thesis: Interactive and Verifiable Web Service Composition, Reformulation, and Adaptation. Recipient of an Iowa State University Graduate Research Excellence Award. Jyotish was supported by a graduate research assistantship in Computer Science funded in part by grants from the National Science Foundation. Initial Employment: Research Scientist, Division of Biomedical Informatics, Mayo College of Medicine, Rochester, Minnesota. Current Employment: Inaugural dean of the School of Technology for Public Health, Arizona State University.

- 31. **Dae-Ki Kang** (Computer Science, Iowa State University). Ph.D., 2007. Abstraction, Aggregation, and Refinement Strategies for Machine Learning. Dae-Ki was funded by a Teaching assistantship from the Department of Computer Science and a Research assistantship funded by the National Science Foundation. Current Employment: Associate Professor, Department of Computer Engineering, Dongseo University, Pusan, Korea.
- 32. **Jun Zhang** (Computer Science). Ph.D., 2005. Ontology Aware Learning Algorithms. Recipient of an Iowa State University Graduate Research Excellence Award. Jun was supported in part by research assistantship funded by a grant from the National Science Foundation and a teaching assistantship from the ISU Department of Computer Science. Initial Employment: Research Scientist, Fair Isaac, San Diego. Current Employment: Vice President of Data Science and Machine Learning, Traceable.
- 33. **Changhui Yan** (Bioinformatics and Computational Biology, Iowa State University; with Drena Dobbs). Ph.D., 2004. Computational Approaches to Prediction of Protein-Protein, Protein-DNA and Protein-RNA Interfaces. 2005. Recipient of an Iowa State University Graduate Research Excellence Award. Changhui was supported by a Plant Sciences Fellowship and research assistantships funded by the ISU Graduate College and a grant from the National Institutes of Health. Initial Employment: Assistant Professor of Computer Science, Utah State University. Current position: Professor of Computer Science, North Dakota State University.
- 34. Doina Caragea (Computer Science, Iowa State University). Ph.D., 2004. Learning Classifiers from Semantically Heterogeneous, Distributed, Autonomous Data Sources. 2004. Recipient of an Iowa State University Graduate Research Excellence Award. Initial Employment: Research Associate, Center for Computational Intelligence, Learning, and Discovery, Iowa State University. Current position: Professor of Computer Science, Kansas State University.
- 35. **Jihoon Yang** (Computer Science, Iowa State University). Ph.D., 1999. Learning Agents for Information Retrieval and Knowledge Discovery, 1999. Initial Employment: Research Scientist, Information Sciences Laboratory, Hughes Research Laboratory, Malibu, CA. Current Employment: Professor of Computer Science, Sogang National University, Korea.
- 36. Karthik Balakrishnan (Computer Science, Iowa State University). Ph.D., 1998. Biologically Inspired Computational Structures and Processes for Autonomous Agents and Robots, Recipient of an Iowa State University Graduate Research Excellence Award. Initial Employment: Senior Research Scientist, Datamining Group, Allstate Research and Planning Center. Current Position: Chief AI and Analytics Officer, Cover Whale.
- 37. Rajesh Parekh (Computer Science, Iowa State University). Ph.D., 1998. Recipient of an Iowa State University Graduate Research Excellence Award. Machine Learning of Automata and Neural Network Pattern Classifiers, 1998. Initial Employment: Senior Research Scientist, Data mining Group, Allstate Research and Planning Center, Menlo Park, CA. USA. Current position: Vice President of AI/ML, Intuit.
- 38. Chun-Hsien Chen (Computer Science, Iowa State University). Ph.D., 1997. Neural Architectures for Knowledge Representation and Inference, 1997. Initial Employment: Research Scientist, Advanced Technology Center, Computer and Communication Research Laboratories, Industrial Technology Research Institute, Taiwan. Current Employment: Associate Professor, Department of Information Management, Chang Gung University, Taiwan.
- 39. Armin Mikler (Computer Science, Iowa State University; with Johnny Wong), Ph.D., 1995. Quo Vadis A Framework for Intelligent Routing in Large Communication Networks. Initial Employment: Research Associate, Scalable Computing Laboratory, DOE Ames Lab, Ames, Iowa. Current Position: Professor and Chair of Computer Science, Georgia State University, USA.

Current Ph.D. Students

- 1. **Neil Ashtekar,** Computer Science and Engineering, Pennsylvania State University. Interests: Machine Learning, Causal Inference. Expected Graduation: Spring 2025. Neil is supported in part by a research assistantship funded by the National Science Foundation.
- 2. **Sahar Hanifi,** Informatics, Pennsylvania State University. Interests: Biomedical data Sciences, Machine Learning, Causal Inference. Expected Graduation: Spring 2025. Sahar is supported in part by a research assistantship funded by the National Science Foundation.
- 3. **Zehao Liu,** Informatics, Pennsylvania State University. Interests: Machine Learning, Causal Inference. Expected graduation: Spring 2028. Zehao is supported in part by a research assistantship funded by the National Science Foundation.
- 4. **Naixin Zhang,** Informatics, Pennsylvania State University. Interests: Machine Learning, Causal Inference. Expected graduation: Spring 2028. Naixin is supported in part by a research assistantship funded by the National Science Foundation.
- 5. **Jingxi Zhu,** Informatics, Pennsylvania State University. Interests: Machine Learning, Causal Inference. Expected graduation: Spring 2028. Jingxi is supported in part by a research assistantship funded by the National Science Foundation.
- 6. **Abhishek Dalvi,** Computer Science and Engineering, Pennsylvania State University. Interests: Machine Learning, Causal Inference. Expected Graduation; Spring 2025. Abhishek is supported in part by a research assistantship funded by the National Science Foundation.
- 7. **Duohan Zhang** (joint with Hadi Hosseini), Informatics, Pennsylvania State University Interests: Multi-agent systems, Machine Learning, Causal inference. Expected graduation: Spring 2028.
- 8. **Weijieying Ren,** Informatics, Pennsylvania State University. Interests: Machine Learning. Big Data Analytics. Longitudinal Data Analysis. Expected Graduation: Spring 2026. Weijieying is funded in part by a research assistantship funded by a grant from the National Science Foundation.
- 9. **Yalda Fazlalizadeh,** Informatics, Pennsylvania State University. Interests: Machine Learning. Expected graduation: Spring 2025. Yalda is supported by a research assistantship funded by Volvo and in part by a teaching assistantship in the College of IST.
- 10. **Hamed Mahdavi** (joint with Mehrdad Mahdavi), Computer Science and Engineering, Pennsylvania State University. Interests: Machine Learning, Optimization.
- 11. **Haya Alshayji,** (joint with Paul Griffin), Industrial and Manufacturing Systems Engineering, Pennsylvania State University. Interests: Understanding Health Disparities using Big Data.
- 12. Teng Xiao, Informatics. Interests: Deep learning. Expected graduation: Spring 2025.
- 13. **Huaisheng Zhu,** Informatics. Interests: Deep learning, scientific discovery. Expected graduation: Spring 2025

PhD Students Currently on Leave.

- 14. **David Foley,** Informatics (**on leave**), Pennsylvania State University. Interests: Biomedical Data Sciences, Longitudinal Data Analysis. Expected Graduation: Spring 2023. David was supported in part by an NIH- funded BD2K Predoctoral Fellowship in Biomedical Data Sciences and was supported by an Endowed Professorship held by Vasant Honavar.
- 15. **Yong Jung,** Bioinformatics and Genomics (**on leave**), Pennsylvania State University. Interests: Bioinformatics. Expected graduation: Spring 2024. Yong was supported in part by a research assistantship funded by the National Science Foundation. Currently working full time.

16. **Thanh Le**, Informatics (**on leave**), Pennsylvania State University. Interests: Machine Learning, Big Data Analytics, Biomedical Informatics. Expected graduation: Fall 2024. Thanh was supported by a research assistantship funded by the Center for Big Data Analytics and Discovery Informatics. Currently working full time, leading a startup.

Major Professor, M.S.

Current M.S. Students

1. Aayush Changani, Computer Science and Engineering, Pennsylvania State University, 2025

M.S. Graduates

- 1. Rishabh Bhatt, Computer Science and Engineering, Pennsylvania State University, 2022.
- 2. Erman Tatar, Computer Science and Engineering, Pennsylvania State University. M.S. 2022.
- 3. Rahul Katiki, Computer Science and Engineering, Pennsylvania State University. M.S. 2021.
- 4. **Cheng-Kai Chen**, (Computer Science and Engineering), Pennsylvania State University. Comparative analyses of networks. M.S. 2020.
- 5. **Mayank Garg** (Computer Science and Engineering), Pennsylvania State University; Predicting energy efficiency of batteries. With Dan Kifer. M.S. 2017.
- 6. **Yiming Zhang** (Bioinformatics & Computational Biology, Iowa State University; with Volker Brendel), M.S. 2014.
- 7. **Sateesh Kodavalli** (Computer Science, Iowa State University). M.S., 2010. Extensible Problem Specific Tutor (xPST): Easy Authoring of Intelligent Tutoring Systems.
- 8. **Bhavesh Sanghvi** (Computer Science, Iowa State University). M.S., 2010. Identifying and eliminating inconsistencies in mappings across hierarchical ontologies. Current Employment: Microsoft.
- 9. **Sushain Pandit** (Computer Science, Iowa State University), M.S., 2010. Ontology-guided extraction of structured information from unstructured text: Identifying and capturing complex relationships. Current Employment: IBM.
- 10. **Tim Alcon** (Bioinformatics & Computational Biology; with Heather Greenlee). Using a Seed- Network to Query Multiple Large-Scale Gene Expression Datasets from the Developing Retina in Order to Identify and Prioritize Experimental Targets. Tim was supported by a Multidisciplinary Graduate Education and Training (MGET) fellowship funded by the USDA.
- 11. Lucas Bonansea (Human-Computer Interaction; with Stephen Gilbert), 2009. 3-d hand gesture recognition.
- 12. **Flavian Vasile** (Computer Science, Iowa State University), 2008. Uncovering the structure of hypergraphs through tensor decomposition: An application to folksonomy analysis. Flavian was supported in part by a teaching assistantship in Computer Science, Iowa State University. Current Employment: Software Engineer, Yahoo! Inc.
- 13. **Oksana Kohutyuk** (Computer Science, Iowa State University), 2007. Thesis: Retina Workbench: Database and software tools for comparative analysis and querying of gene and protein networks. Oksana was supported by a research assistantship funded by the National Institutes of Health and a teaching assistantship in Computer Science, Iowa State University. Current position: Software Engineer, Cisco.
- 14. **Charles Giesler** (Computer Science, Iowa State University), A Java Reinforcement Learning Module for the Recursive Porous Agent Simulation Toolkit: Facilitating study and experimentation with reinforcement learning in social science multi-agent simulations. 2003. Current Position: Lawrence

Livermore Labs.

- 15. **Anna Atramentov** (Computer Science, Iowa State University), A Multi-Relational Decision Tree Learning Algorithm – Implementation and Experiments. 2003. Current position: Ph.D. Student, University of Illinois at Urbana-Champaign
- 16. Zhong Gao (Bioinformatics, Iowa State University), Genome wide recognition of tumor necrosis factor (TNF) like ligands in human and Arabidopsis genomes: A structural genomics approach. 2003 Initial Employment: Post-doctoral fellow, The Center for Cardiovascular Bioinformatics and Modeling, Johns Hopkins University.
- 17. Jaime Reinoso-Castillo (Computer Science, Iowa State University), Ontology-Driven Query-Centric Information Integration from Heterogeneous, Distributed, Autonomous Data Sources for Computer Assisted Scientific Discovery. 2002. Initial Employment: Universidad Javeriana, Colombia.
- Hector Leiva (Computer Science, Iowa State University), Learning Classifiers from Relational Data.
 2002. Initial Employment: Research Scientist, Research Scientist, Universidad Nacional de San Luis.
 Argentina.
- 19. **Xiaosi Zhang** (Bioinformatics, Iowa State University), Identification of Functionally Related Genes from Gene Expression Data. 2002.Initial Employment: Papajohn Center for Entrepreneurship, Ames, Iowa.
- 20. **Xiangyun Wang** (Bioinformatics, Iowa State University), Data Mining Approach to Discovery of Protein Sequence-Structure-Function Relationships. 2002. Initial Employment: Astra-Zeneca Inc.
- 21. **Kent Vander Velden** (Bioinformatics, Iowa State University, joint supervision with Gavin Naylor), Spatial Clustering of Differences in Measured Homoplasy with Respect to Protein Structure. 2002. Initial Employment: Pioneer Hi-Bred, Inc.
- 22. **Neeraj Koul** (Computer Science, Iowa State University), Clustering with Semi-Metrics, 2001. Initial Employment: Motorola.
- 23. **Dake Wang** (Computer Science, Iowa State University), Data-Driven Generation of Decision Trees for Motif-Based Assignment of Protein Sequences to Functional Families., 2001. Initial Employment: Lumicyte, Inc. Current Employment: Genentech, Inc.
- 24. **Rushi Bhatt** (Computer Science, Iowa State University), Spatial Learning and Localization: A Computational Model and Behavioral Simulations, 2001. Ph.D. Program, Boston University.
- 25. **Fajun Chen** (Computer Science, Iowa State University), Learning Information Extraction Patterns from Text, 2000. Initial Employment: Ericsson.
- 26. **Tarkeshwari Sharma** (Computer Science, Iowa State University), Agent Toolkit for Distributed Knowledge Networks, 2000. Initial Employment: Motorola, Inc.
- 27. **Asok Tiyyagura** (Computer Science, Iowa State University), Alternative Criteria for Association Rule Mining, 2000. Cisco Systems, Inc.
- 28. Di Wang (Computer Science, Iowa State University), 1997. Mobile Agents for Information Retrieval.
- 29. **Shane Konsella** (Computer Science, Iowa State University), 1996. Trie Compaction Using Genetic Algorithms. Initial Employment: Hewlett-Packard.
- 30. **Karthik Balakrishnan** (Computer Science, Iowa State University), 1993. Faster Learning Approximations of Backpropagation by Handling Flat-Spots. Continued as a Ph.D. student.
- 31. **Jayathi Janakiraman** (Computer Science, Iowa State University), 1993. Adaptive Learning Rate for Increasing Learning Speed in Backpropagation Networks. Initial Employment: Motorola.
- 32. **Priyamvadha Thambu** (Computer Science, Iowa State University), 1993. Automated Knowledge-Base Consistency Maintenance in an Evolving Intelligent Advisory System. Initial Employment: Inference Corporation.

- 33. **Rajesh Parekh**, 1993 (Computer Science, Iowa State University). Efficient Learning of Regular Languages Using Teacher-Supplied Positive Examples and Learner-Generated Queries. Continued as a Ph.D. student.
- 34. **Richard Spartz**, 1992 (Computer Science, Iowa State University). Speeding Up Backpropagation Using Expected Source Values. Initial Employment: IBM.

Member of Graduate Program of Study (Thesis) Committees Ph.D. Committees

- 1. Rupesh Prajapati, Informatics, PSU, 2023
- 2. Vijay Kumar Pounraja, Bioinformatics and Genomics, PSU, 2021
- 3. Yanling Li, Human Development and Family Studies, PSU, 2021
- 4. Juxihong Julaiti, Industrial and Manufacturing Systems Engineering, PSU, 2021
- 5. Chen Liang, Information Sciences and Technology, PSU, 2018
- 6. Yafei Wang, Information Sciences and Technology, PSU, 2017
- 7. Moojan Gafurian, Information Sciences and Technology, PSU, 2017
- 8. Rabah Al-Zaidy, Computer Science and Engineering, PSU, 2017
- 9. Mehdi Bagherzadeh, Computer Science, ISU, 2016
- 10. Seifu Chonde, Industrial Engineering, PSU, 2016
- 11. Robert Dyer, Computer Science, ISU, 2013
- 12. Scott Boyken, Bioinformatics and Computational Biology, ISU, 2013
- 13. Haitao Cheng, Bioinformatics and Computational Biology, ISU, 2013
- 14. Ataur Katebi, Bioinformatics and Computational Biology, ISU, 2013
- 15. Jivko Sinapov, Computer Science, ISU, 2013
- 16. Ru He, Computer Science, ISU, 2013
- 17. Chris Strasburg, Computer Science, ISU, 2013
- 18. Zack Oster, Computer Science, ISU, 2013
- 19. Yao Fu, Bioinformatics and Computational Biology, ISU, 2013
- 20. Oliver Couture, Genetics, ISU, 2011
- 21. Tu-Liang Lin, Computer Science, ISU, 2011
- 22. Brian Patterson, Computer Science, ISU, 2011
- 23. Aimin Yan, Bioinformatics and Computational Biology, ISU, 2011
- 24. Deepak Reyon, Bioinformatics and Computational Biology, ISU, 2011
- 25. Scott Broderick, Material Science and Engineering, ISU, 2009
- 26. Changsung Kang, Computer Science, ISU, 2008
- 27. Jeff Sander, Bioinformatics and Computational Biology, ISU, 2008
- 28. Lei Yang, Bioinformatics and Computational Biology, ISU, 2008
- 29. Facundo Bromberg, Computer Science, ISU, 2007
- 30. Jae-Hyung Lee, Bioinformatics and Computational Biology, ISU, 2007

- 31. Yu Cao, Computer Science, ISU, 2007
- 32. Laura Hecker, Neuroscience, ISU, 2007
- 33. Oleksiy Atramentov, Physics, ISU, 2006
- 30. Xiaonan Li, Industrial and Manufacturing Systems Engineering, ISU, 2006
- 31. Di Wu, Bioinformatics and Computational Biology, ISU, 2006
- 34. Yungok Ihm, Bioinformatics and Computational Biology, ISU, 2004
- 35. Cizhiong Zhang, Bioinformatics and Computational Biology, ISU, 2004
- 36. Zhong Zhang, Electrical and Computer Engineering, ISU, 2004
- 37. Haibo Cao, Physics, ISU, 2003
- 38. Brooke Peterson, Genetics, 2003
- 39. Marybeth Gurski, Computer Science, 2001
- 40. Guy Helmer, Computer Science, ISU, 2001
- 41. Robi Polikar, Electrical and Computer Engineering, ISU, 2001
- 42. Vincent Van Acker, Electrical and Computer Engineering, ISU, 2000
- 43. Chun-Fu Chen, Economics, ISU, 1999
- 44. Maria Victoria Bascunana, Chemical Engineering, ISU, 1999
- 45. Guozhong Zhou, Electrical and Computer Engineering, ISU, 1998
- 46. Cheng-Chi Tai, Electrical and Computer Engineering, ISU, 1998
- 47. James Lathrop, Computer Science, ISU, 1997
- 48. Krishna Dhara, Computer Science, ISU, 1997
- 49. Babak Fourouraghi, Computer Science, ISU, 1995
- 50. Timothy Wahls, Computer Science, ISU, 1995
- 51. Chang-Chun Tsai, Industrial and Manufacturing Engineering, ISU, 1995
- 52. Sonmez Rifat, Civil and Constructional Engineering, ISU, 1995
- 53. Richa Agrawala, Computer Science, ISU, 1994
- 54. Bamshad Mobasher, Computer Science, ISU, 1994
- 55. Hun Kang, Electrical and Computer Engg., ISU, 1993

M.S. Committees

- 1. Sandeep Krishnan, Computer Science, ISU, 2009
- 2. Zack Oster, Computer Science, ISU, 2009
- 3. Georgi Batinov, Economics, ISU, 2007
- 4. Inya Nlenanya, Agricultural Engineering, ISU, 2005
- 5. Jing Xu, Psychology, ISU, 2005
- 6. Suxing Cheng, Computer Science, ISU, 2005
- 7. Kyongryun Lee, Computer Science, ISU, 2005

- 8. Haitao Cheng, Computer Science, ISU, 2004
- 9. Patricia Lonosky, Genetics, ISU, 2002
- 10. Mallika Bachan, Statistics, ISU, 2002
- 11. Melinda Vander Velden, Electrical and Computer Engineering, ISU, 2002
- 12. Jeremy Patterson, Computer Science, ISU, 2001
- 13. Sa Lin, Computer Science, ISU, 2001
- 14. Vijay Viswanathan, Electrical and Computer Engineering, ISU, 2001
- 15. Fengmei Liu, Computer Science, ISU, 2001
- 16. Xinhua Dong, Computer Science, ISU, 2001
- 17. Mark Slagell, Computer Science, ISU, 2001
- 18. Hao Dong, Computer Science, ISU, 2001
- 19. Jun Li, Computer Science, ISU, 2001
- 20. Thai-Tin Huang, Computer Science, ISU, 2000
- 21. Ran Liu, Computer Science, ISU, 2000
- 22. Xumei Lu, Computer Science, ISU, 2000
- 23. Nanchang Yang, Computer Science, ISU, 2000
- 24. Peng Han, Botany, ISU, 1999
- 25. Jeffrey Yakey, Computer Science, ISU, 1999
- 26. Sunitha Kothapalli, Electrical Engineering, ISU, 2000
- 27. Raghunandan Havaldar, Computer Science, ISU, 1998
- 28. Guy Helmer, Computer Science, ISU, 1998
- 29. Ngee Jenn Lee, Mechanical Engineering, ISU, 1998
- 30. Laura Nelson, Computer Science, ISU, 1998
- 31. Jibin Xiang, Computer Science, ISU, 1998
- 32. Venkat Naganathan, Computer Science, ISU, 1998
- 33. Dean Stevens, Computer Science, ISU, 1998
- 34. Prashant Pai, Computer Science, ISU, 1998
- 35. Abhinav Rawat, Nuclear Engineering, ISU, 1998
- 36. Rishi Nayar, Computer Science, ISU, 1997
- 37. Marcie Goodman, Computer Science, ISU, 1997
- 38. Jon Schultze-Hewett, Computer Science, ISU, 1997
- 39. Chin Khor, Mechanical Engineering, ISU, 1997
- 40. Qiang-lin Zhao, Computer Science, ISU, 1996
- 41. Chi-Chuan Chen, Agricultural Engineering, ISU, 1996
- 42. Mahesh Subramaniam, Computer Science, ISU, 1996
- 43. Glen Holt, Computer Science, ISU, 1996

- 44. Niranjan Vaidya, Computer Science, ISU, 1996
- 45. Thirumalai Anandapillai, Industrial and Manufacturing Engineering, ISU, 1995
- 46. Thomas DeWulf, Electrical Engineering, ISU, 1994
- 47. Raghav Trivedi, Computer Science, ISU, 1994
- 48. Arun Barboza, Computer Science, ISU, 1994
- 49. Brian Schmidt, Electrical and Computer Engineering, ISU, 1993
- 50. Brian Peterson, Computer Science, ISU, 1992
- 51. Salim Chandani, Industrial and Manufacturing Engineering, ISU, 1992
- 52. Prerana Vaidya, Computer Science, ISU, 1991
- 53. James Wittry, Computer Science, ISU, 1991
- 54. Srinivas Boddu, Electrical Engineering, ISU, 1991
- 55. Simanta Mitra, Computer Science, ISU, 1991

UNDERGRADUATE STUDENT RESEARCH SUPERVISION

Supervisor, Undergraduate Honors Project

- 1. Andres De la Fuente (2018-2019) Topics in Reinforcement Learning. PSU.
- 2. Benjamin Myers (2016-2017). Topics in Machine Learning. PSU.
- 3. Preston Soeperanto (2016-2017). Topics in Machine Learning. PSU
- 4. Dom Mirabile (2014). Topics in Machine Learning. PSU.
- 5. Oksana Yakhneko (2003-2004). Topics in Machine Learning. ISU
- 6. Eric Barsness (1993), An Object-Oriented Implementation of a Genetic Algorithms Testbed. ISU
- 7. Daniel Graves (1992), Parallel Architectures for Artificial Intelligence. ISU

Supervisor, Undergraduate Research

- 1. Letao Qi, Iowa State University, 2012-2013. Graduate school: Rice University.
- Lionel Barrow, Bard College, Participant, Summer Institute in Bioinformatics and Computational Systems Biology, ISU 2010
- 3. Kim Eue, Iowa State University, Summer Research Student, 2010
- 4. Kiran Gustavson, Iowa State University, Summer Research Student, 2010
- 5. Ryan Pendergast, College of the Holy Cross, Participant, Summer Institute in Bioinformatics and Computational Systems Biology, ISU, 2010
- 6. Marjie Volk, Iowa State University, Undergraduate Research Assistant, ISU, 2010-2011
- 7. Katie Wilkins, Case Western Reserve University, Participant, Summer Institute in Bioinformatics and Computational Systems Biology, ISU 2009
- 8. Casey Oliver, Penn State University, Participant, Summer Institute in Bioinformatics and Computational Systems Biology, ISU 2009
- 9. Susan Koons, Texas A&M University, Participant, Summer Institute in Bioinformatics and Computational Systems Biology, ISU 2009.
- 10. Kevin Yang, Cornell University, Summer Research Student, ISU. 2008.
- 11. Tyson Williams, Undergraduate Research Assistant, ISU 2007-2008.
- 12. David Gemperline, Participant, Summer Institute in Bioinformatics and Computational Systems Biology, 2007. ISU

- 13. Keith Callenberg, Participant, Summer Institute in Bioinformatics and Computational Systems Biology, 2007. ISU. Graduate School: Carnegie Mellon University.
- 14. Remy Younes, Undergraduate Research Assistant. Topics in Data Integration. 2007. ISU
- 15. Matt Miller, Topics in Learning Classifiers from Distributed Data, 2006-2007. ISU (Graduate School: MIT)
- 16. John Leacox, Topics in Data Integration, 2006. ISU
- 17. Peter Wong, Topics in Collaborative Ontology Development, 2006. ISU
- 18. Ryan Bruce (2004), Topics in Bioinformatics, ISU
- 19. Cody Pfau (2003). Topics in Data Mining. ISU
- 20. Amy Nienaber (2003). ISU. Computational Discovery of Protein-Protein Interactions
- 21. Matthew Beard (2003). Computational Discovery of Protein-Protein Interactions
- 22. Diane Schroeder (2001-2002) Data Mining Approaches to Discovery of Protein Sequence Function Relationships, ISU (Graduate School: Stanford University)
- 23. Kent Vander Velden (1998-1999), Protein Structure Prediction. ISU (Graduate School: Bioinformatics, Iowa State University)
- 24. Jeremy Ludwig (1996-1997), Topics in Neural Computing. ISU (Graduate School: U. Pittsburgh).
- 25. David DeYoe (1996-1997), Topics in Cognitive Modelling. ISU
- 26. Carl Pecinovsky (1996-1997), Constructive Neural Network Learning Algorithms. ISU
- 27. Brian Walenz, Topics in Genetic Algorithms (Graduate School: Computer Science, University of New Mexico). ISU
- 28. Gabriel Ki (1996-), Situated Robotics. ISU
- 29. Todd Lindsey (1995-96), Constructive Neural Network Learning Algorithms. ISU
- 30. Jouko Rytilahti (1994), Explorations in Evolutionary Algorithms. ISU
- 31. Leigh McMullen (1993), Adaptive Game-Playing Programs. ISU

Mentor, Freshman Honors Study

- 1. Marjie Volk (2010) Topics in Machine Learning. ISU
- 2. Jeffrey Schroeder (1997) Topics in Artificial Intelligence. ISU
- 3. Matthew Potter (1997) Topics in Artificial Intelligence. ISU
- 4. Brian George (1994), Topics in Neural Computing. ISU
- 5. Adam Johnson (1994), Topics in Neural Computing. ISU
- 6. Marcus Ryan (1993), Topics in Artificial Intelligence. ISU

PRE-COLLEGE STUDENT RESEARCH SUPERVISION

Mentor (for pre-college students)

- 1. Eric Solan, Nic Dayton, Luke Rolfes, and Julian Sheldahl. Animus Facticius. Adventures in Supercomputing (1998) project. First Place.
- 2. Sara Karbeling et al., A Computational Model of Animal Spatial Learning Adventures in Supercomputing (1998) project.
- 3. Sara Karbeling, Kellan Brumback, Anna Keyte, and Angel Sherif (1997), Lateral Inhibition and Sensory Processing in the Limulus Polyphemus Eye, Adventures in Supercomputing (AIS-97) project. First place in Iowa, and Second Place in the National Competition.
- 4. Stephen Lee (1993), Topics in Neural Computing.
- 5. John Farragher (1992), Topics in Neural Computing.

6. Peter Luka (1991), Topics in Neural Computing.

SPONSORSHIP OF VISITING RESEARCHERS

- 1. Morteza Jaderyan, Visiting PhD Student, Bu Ali Sina University, Iran. 2016-2017.
- 2. Professor Jinlong Hu, South China University of Technology, 2016-2017.
- 3. Professor Jihoon Yang, Sogang University, Korea, 2008.
- 4. Oswaldo Velesz-Langs, Madrid Polytechnic University, Madrid, Spain. 2003.
- 5. Professor Yigon Kim (on Sabbatical from Yosu National University, Yosu, Korea 2000-2001) Data Mining and Knowledge Discovery.
- 6. Professor Mok Dong Chung (on Sabbatical from Pukyong National University, Korea, 1999-2000) Agent-based systems and knowledge-based systems.
- 7. Olivier Bousquet (from Ecole Polytechnique, France, 1997) Topics in Cognitive Modeling and Robotics.
- 8. Codrin Nichitiu (from ENS Lyon, France, Summer 1996), Topics in Machine Learning.
- 9. Dimitri Kotchetkov (Visitor from Ukraine, Summer 1996), Topics in Robotics.
- 10. Vadim Kirillov (Fullbright Scholar from Ukraine, 1995), Constraint-based Reasoning under uncertainty.

TEACHING STATEMENT Teaching Philosophy

My teaching philosophy is best summed up by a quote from Joseph Chesterton: "The Foundation of teaching is research; and the object of research is teaching, that is, the dissemination of knowledge."

In my view, teaching is an integral and extremely rewarding part of academic life. I like to teach what I like to learn. It is hard to top the joy of grasping a new idea or solving an unsolved problem for the very first time. I subscribe to John Dewey's view of education: "Education is not preparation for life; education is life itself." For me, teaching is not just about communicating what is thought to be known but cultivating the ability in students to challenge the current state of knowledge, and to venture beyond the current frontiers of knowledge into the unknown, on a life-long journey of learning and discovery. As Richard Dann remarked, "He who dares to teach must never cease to learn." Most of my curriculum development and teaching activities in computer science strongly complement and are sustained by an active research program.

In my view, teaching computer science is not *just* about teaching students to be competent programmers or creators and users of sophisticated software tools; it is about introducing computer science as a profoundly interesting scientific discipline. Computer science provides us with the best language we have so far – the language of algorithms – precise recipes for describing processes that manipulate information – for modeling biological, cognitive, and social phenomena – just as calculus provided Newton and his successors with a language for modeling physical phenomena.

In my view, teaching Data Science or Informatics is not *just* about teaching students to use or even design sophisticated tools for data analyses; it is about instilling an appreciation for the promise as well as pitfalls of data-driven analyses, an understanding the mathematical and statistical foundations of data science; mastery of sound scientific and engineering approaches and ethical principles in applying data science methods and tools in real-world settings.

In my view, teaching Artificial Intelligence is not *just* about teaching students to develop "intelligent systems"; It is about fostering a deep appreciation of the interdisciplinary intellectual, philosophical, scientific, engineering underpinnings of Artificial Intelligence and its promise, potential, pitfalls and societal impact across many areas of human endeavor; and mastery of the scientific and engineering approaches for designing effective artificial intelligence systems that conform to ethical principles and

societal values.

I am excited about educating the next generation of scientists, engineers, and practitioners to realize the promise and potential of data and algorithmic abstractions to help us understand biological, cognitive, and social phenomena and to address major scientific and societal challenges.

Teaching Style

My personal teaching style involves:

- (a) Engaging students so that they become active participants in the learning process rather than passive observers ("What I hear, I forget. What I see, I remember. What I do, I understand" Confucius).
- (b) Setting the stage for the topic of study We learn what we *almost* already know. Hence, I find it useful to introduce a complex idea or a new topic or through a succession of smaller steps, establishing their connection with familiar topics, each building on what my students already know.
- (c) Setting challenging yet realistic goals In my experience, students respond best, and learn most, from learning goals that are both challenging and achievable. Assignments that are trivial are boring. Assignments that are excessively difficult can be frustrating and intimidating.
- (d) Letting students make mistakes and learn from them. Exploration and experimentation are essential to learning and discovery and learning what does not work (and why) is as important as learning what works (and why).
- (e) Accommodating different learning styles Kolb identifies several learning styles. Some learn best from observations and examples; others by acquiring general principles and knowledge of how to apply them in specific situations; others by deducing and discovering general principles or theories; and yet others by doing – that is, by trying things, making mistakes, and learning from them. I find it useful to develop course materials that exercise multiple learning styles.
- (f) Incorporating discussion of ethical considerations and societal impact of data science and artificial intelligence methods, tools, and applications.

Teaching and Curriculum Development Experience

Over the past 30 years, I have designed, developed, and taught undergraduate as well as graduate courses and seminars in artificial intelligence, intelligent agents and multi-agent systems, data sciences, causal inference, machine learning, data mining and knowledge discovery, neural and evolutionary computation, computational learning theory, bioinformatics, and computational biology. The material covered in the courses is chosen with an emphasis on concepts that are likely to have a lasting impact on the discipline in the years to come. In addition to introducing students to a core body of knowledge in the areas of study, these courses present such knowledge in the broader context of computer science as an intellectual discipline and to develop the students into creative thinkers and problem-solvers, be it in academic research or advanced technology development.

In addition to developing and teaching courses, I have had substantial experience developing new curricula and programs.

As a founding member and member of the Data Sciences Undergraduate Program Task force at Pennsylvania State University, I have co-led the development of an undergraduate program in Data Sciences, a joint initiative of the College of Information Sciences and Technology, School of Electrical Engineering and Computer Science, and the Department of Statistics. The program is organized into three tracks, one focused on Big Data Systems and Algorithms, one on Statistical Foundations, and one on Applied Data Sciences. While the tracks share a set of core courses in the foundations of data sciences, they allow students to specialize in the computational, statistical, or applied aspects of data sciences. Electives allow students to get exposure to an application domain of their choosing (e.g., Social Sciences, Life Sciences, etc.).

I have co-led the development of an undergraduate degree program in Artificial Intelligence at Penn State. The program is designed to equip students with not only foundational and technical aspects of artificial intelligence, but also, ethical, and societal considerations involved in responsible application of AI to the benefit of humanity.

I have also led the development of the curriculum for an NIH-funded PhD program in Biomedical Data Sciences at Penn State. The core curriculum includes courses in Machine Learning, Statistics, Scalable Methods, and Data Privacy and Ethics, with advanced electives drawn from graduate courses in Data Sciences from multiple disciplines including Computer Science, Statistics, and Information Sciences and Technology. Biomedical Sciences electives offer exposure to one or more relevant area of life sciences, e.g., genomics, population health, etc.

I have also co-led the development of the curriculum for a Masters Program in Data Sciences at Penn State. The program is aimed at PhD students in a variety of disciplines who are interested in pursuing a concurrent Masters in Data Sciences to expand their skills in managing and analyzing large and complex data sets in their own disciplines as well as Masters students interested in careers in industry. The program is currently under consideration for implementation at Penn State. I am currently co-leading the development of interdisciplinary undergraduate and Masters degree programs in Artificial Intelligence.

As a founding member of the interdepartmental graduate program in Bioinformatics and Computational Biology (BCB) at Iowa State University, I worked with an interdisciplinary team of biologists to secure an Integrative Graduate Education and Research Training (IGERT) award which helped establish one of the first (and one of the largest, and perhaps one of the strongest Bioinformatics Ph.D. programs in the United States, among universities without medical schools. I have led the development of a set of 4 core courses in Bioinformatics and Computational Biology covering Genome Informatics, Structural Genome Informatics, Functional Genomics, and Systems Biology. I have developed and taught short course modules as part of an NSF-supported Bioinformatics Summer Institute in Bioinformatics and Computational Biology, which has been offered at Iowa State University beginning in fall 2007.

The undergraduate and graduate courses that I have developed and taught over the years introduce students to some of the most challenging topics in computer science – involving the application of concepts and tools from the theory of computation, design and analysis of algorithms, and design of software systems in the construction of *intelligent* artifacts: computer programs that represent and reason with and about knowledge, acquire knowledge from interaction with their environment, and discover and use regularities from data.

I have developed and taught a combined upper level undergraduate and introductory graduate course in Artificial Intelligence with emphasis on fundamental problems and approaches in the design of intelligent agents. This course is aimed at introducing students to the foundations of artificial intelligence, including representing and reasoning with and about knowledge, problem solving, decision making, planning and machine learning. This course has been popular with graduate and senior undergraduate students in Computer Science, Engineering, and related disciplines.

I have developed and taught an undergraduate introductory course in machine learning, that introduces students to the theory and practice of machine learning. The course covers the underlying mathematical and statistical ideas, representative machine learning algorithms, and their practical applications. This course serves as a core course for the Data Sciences undergraduate program.

I have developed and taught both introductory and advanced graduate courses in Machine Learning. The introductory course provides a unified introduction to the principles, techniques, and applications of

Machine Learning. It covers rigorous statistical and algorithmic foundations of machine learning and a suite of representative algorithms for learning predictive models from data. The course is designed to help students gain a broad understanding of the current state of the art in machine learning, adapt and apply machine learning approaches to real- world applications (e.g., in computational biology, semantic web), and begin to conduct original research in machine learning. Advanced courses have focused on topics such as Computational Learning Theory, Deep Learning, Kernel Methods, Gaussian Processes, among others.

I have developed and taught a graduate course on Foundations of Causal Inference. The course provides a unified introduction to both Rubin and Pearl frameworks for causal inference, including the assumptions under which it is possible to estimate causal effects from observational and experimental data, learn causal models, identify, and control for confounders, generalize causal discoveries across related yet different settings, and the applications of causal models across disparate scientific disciplines.

I have developed and taught a graduate course on Data Science for Researchers, Scholars, and Practitioners, which provides a broadly accessible yet rigorous introduction to descriptive, predictive, and causal data science methods, tools, and their principled applications across diverse disciplines. This course is popular with graduate students from a broad range of PhD programs beyond Informatics, including Behavioral and Cognitive Sciences, Social Sciences, Physical Sciences, Biomedical and Health Sciences, Engineering, Business, Life Sciences, Learning Sciences, among others. In addition to mastering the key concepts behind the methods, the students acquire practical experience with applying the methods to answer scientific questions of interest in their respective fields using real-world data.

I have developed and taught an undergraduate course on neural computation. Because no textbook on this topic suitable for undergraduate students in Computer Science was available in 1992 when I first offered the course, I developed most of the material for this course in the form of lecture notes some of which were adapted for use in graduate and undergraduate courses in other universities. The course covered computational models of neurons and networks of neurons (neural networks) and neural network learning algorithms.

I have developed and taught a graduate course on intelligent agents and multi-agent systems which draws on material from game theory, knowledge representation and inference, decision theory, contract theory, bargaining theory, and related areas to develop an understanding of fundamental problems in the design of open-ended systems consisting of loosely coupled systems consisting of interacting autonomous entities (information sources, intelligent agents) e.g., the semantic web.

I have developed and taught a graduate course on Causal Inference from Observational and Experimental Data. The course offers a comprehensive coverage of the theoretical underpinnings, and practice of causal inference from observational and experimental data. Randomize control trials; causal inference in the absence of randomized control trials; causal effects and counterfactuals; eliciting causal effects from observations; the Causal Bayesian Network framework for causal inference - do-calculus, identifiability of causal effects from observations and experiments; the Potential Outcomes framework for causal inference - counterfactual inference; the relationship between the Potential Outcomes and Causal Bayes Networks; and learning causal models from observations and experiments. The course includes a principled treatment of confounders and practical approaches to cope with them. Additional topics covered include mediation analysis; causal transportability, selection bias, and applications of causal inference in uncovering algorithmic bias, explaining black box predictive models, etc.

I have developed an introductory first-year course in artificial intelligence for a broad general audience at Penn State university. The course is scheduled to be taught for the first time in spring of 2024. The course aims to offer a broad and accessible introduction to the interdisciplinary roots of AI, the recent advances in AI, the promise and potential of AI as well as the potential risks of AI, to enable students from diverse backgrounds to meaningfully engage in societal dialog about responsible uses of AI.

I have developed and taught a course on Foundations of Informatics aimed at graduate students in

Informatics who are drawn from diverse disciplinary backgrounds. The course covers the conceptual and theoretical foundations of informatics, with particular emphasis on the role of computational or algorithmic abstractions in artificial intelligence, cognitive and brain sciences, social, behavioral, and economic sciences, and life sciences, and the humanities. In each case, concrete examples are used to illustrate how fundamental questions in the domain can be translated into algorithmic problems that can then be solved using concepts, methods, and tools of computer science; and how to devise and study algorithmic abstractions of problems in artificial intelligence (e.g., learning and reasoning), cognitive sciences (relating brain activity to behavior), social sciences (rational behavior, collective decision making), life sciences (gene regulation) and the humanities (analysis of cultural artifacts).

I have developed and co-taught a course on Functional Genomics and Computational Systems Biology which is the fourth in a sequence of 4-course core curriculum that I helped develop for the Bioinformatics and Computational Biology graduate program. This course, among the first of its kind, was offered for the first time at ISU in the spring of 2008.

In addition to the regular courses, current research topics are explored in depth in research seminars, which I have organized or co-organized with the help and active participation of my graduate students.

The nature of the material taught in my courses requires a delicate balance between theory and experimentation. In a fast-paced field like computer science in general and artificial intelligence and bioinformatics in particular, the courses must anticipate key developments in the field that are likely to have a long-term impact and provide students with a solid understanding of the fundamentals as well the insight that comes with hands-on experience. Hence, I have invested in efforts to develop the laboratory facilities that are essential to support experiments, exercises, and projects that enhance the students' understanding the material covered in the courses.

To help develop the written and oral communication skills of students, most of my courses require individual or team research projects culminating in a short paper. It has been my experience that team projects promote collaborative learning and problem solving. The projects often serve as vehicles for integrating latest research results into the graduate and undergraduate curriculum. They also provide an opportunity for students to exercise their creativity and explore new solutions to open problems in artificial intelligence. In many instances, such class projects have evolved into thesis research topics or produced results that were eventually published in refereed national and international conferences.

Teaching Interests

I have a strong interest in teaching undergraduate and graduate courses in artificial intelligence, machine learning, bioinformatics, data sciences, causal inference, knowledge representation, semantic web, and related topics. I am very interested in developing and teaching courses that incorporate significant research advances in the relevant disciplines and prepare students to address new research challenges in informatics, scientific discovery, and related areas.

I am also interested in offering focused special topics or seminar courses aimed at students in the undergraduate honors program, and graduate students on topics of current interest.

I enjoy contributing to the development of new graduate and undergraduate programs designed to train a new generation of scientists well-versed in computer and information sciences and the creative and skillful application of information processing approaches to address fundamental scientific problems in biological, agricultural, cognitive, environmental, health, physical and social sciences.

Given an opportunity, I would especially enjoy developing and teaching a course that introduces artificial intelligence, data science or informatics as an intellectual discipline to a broad audience of undergraduates (and graduate students) drawn from across all areas of science, engineering, and the humanities.

Brief Description of Representative Courses Developed and Taught

- Principles of Causal Inference. Graduate course developed and taught at Pennsylvania State University. Causation versus association. Potential outcomes framework for counterfactual inference. Estimation of causal effects from observational data. Causal effects identifiability. Structural causal models. Confounding. Learning causal models from data. Causal effects transportability and related topics.
- Data Science for Researchers, Scholars, and Practitioners. Graduate course developed and taught at Pennsylvania State University. Transdisciplinary foundations of data science. Statistical and algorithmic underpinnings of data science. Descriptive, predictive, and causal data science. Responsible data science practice: Bias, reproducibility, ethic.
- Artificial Intelligence The Very Idea. Undergraduate course developed and taught at Pennsylvania State University. An introductory General Education course introducing Artificial Intelligence to a broad audience of first-year undergraduates with diverse disciplinary interests and backgrounds. The course covers fundamental concepts for AI literacy, as well as the ethical and societal implications of AI technologies. Students will acquire general AI literacy, including: the intellectual roots of AI, the disparate goals of AI, the many types of AI and their applications, the risks, the benefits, and the societal impacts of AI technologies, and how to distinguish AI science from AI science fiction.
- Principles of Artificial Intelligence. Graduate Course developed taught at Iowa State University and Pennsylvania State University. Specification, design, implementation, and selected applications of intelligent software agents and multi-agent systems. Computational models of intelligent behavior, including problem solving, knowledge representation, reasoning, planning, decision making, learning, perception, action, communication, and interaction. Reactive, deliberative, rational, adaptive, learning, and communicative agents. Artificial intelligence programming. Graduate credit requires a research project and a written report. Oral and written reports.
- Foundations of Informatics. Graduate course developed and taught at Pennsylvania State University. The course introduces the power of algorithmic thinking and information processing characterizations of natural and synthetic systems. The world viewed through an algorithmic lens. Review of theories of computation, complexity, information, and communication. Algorithmic abstractions of intelligence; algorithmic abstractions in cognitive and brains sciences; algorithmic abstractions in life sciences; algorithmic abstractions in the social sciences.
- Principles of Machine Learning. Graduate course developed and taught at Iowa State University and Pennsylvania State University. Statistical Learning Theory and Applications (decision theoretic foundations, probabilistic generative models, discriminative models, kernel machines, representative algorithms); Algorithmic Learning Theory and Applications (mistake bound, PAC, Occam, curriculum learning models, representative algorithms); Probabilistic graphical models (Bayesian networks, Markov models, Hidden Markov Models, Latent Variable models, Probabilistic relational models, Stochastic process models, grammars, representative algorithms); Selected topics (multi-instance learning, multi-label learning, multi-relational learning, structured label learning, distributional learning, deep learning, longitudinal learning); Learning predictive models from Big Data (learning from large data, high dimensional data, distributed data, linked data, platforms and tools).
- Machine Learning for Data Science. Undergraduate course developed and taught at Pennsylvania State University. The course introduces students to the principles of machine learning, representative machine learning algorithms, and their applications in the data sciences. Topics covered include principled approaches to classification, clustering, and function approximation, feature selection and dimensionality reduction, performance assessment of

predictive models, relative strengths, and weaknesses of alternative algorithms. Representative machine learning approaches to be covered include: Supervised machine learning methods for classification including Probabilistic generative models (e.g., Naïve Bayes), and their discriminative counterparts (e.g., Logistic regression), Linear Classifiers, Tree-based models (decision trees, random forests), Nearest-neighbor methods, Kernel machines (Support Vector Machines), Neural networks and deep neural networks; Clustering algorithms (K-means, hierarchical, spectral), and function approximation (e.g., neural networks). Students gain hands-on experience with the implementation and applications of machine learning algorithms through programming projects.

- Computational Functional Genomics and Systems Biology. Graduate course developed and taught at Iowa State University. Algorithmic and statistical approaches in computational functional genomics and systems biology. Analysis of high throughput gene expression, proteomics, and other datasets obtained using system-wide measurements. Topological analysis, module discovery, and comparative analysis of gene and protein networks. Modeling, analysis, simulation and inference of transcriptional regulatory modules and networks, protein-protein interaction networks, metabolic networks, cells, and systems: Dynamic systems, Boolean, and probabilistic models. Ontology-driven, network based, and probabilistic approaches to information integration.
- Intelligent Multiagent Systems. Graduate course developed and taught at Iowa State University. Specification, design, implementation, and applications of multi-agent systems. Intelligent agent architectures; infrastructures, languages and tools for design and implementation of distributed multi-agent systems; Multi-agent organizations, communication, interaction, cooperation, team formation, negotiation, competition, and learning. Selected topics in decision theory, game theory, contract theory, bargaining theory, auction theory, and organizational theory. Selected topics in knowledge representation and ontologies. Agent-based systems and the Semantic Web. Applications in distributed intelligent information networks for information retrieval, information integration, inference, and discovery from heterogeneous, autonomous, distributed, dynamic information sources.
- Advanced Topics in Computational Models of Learning. Graduate course developed and taught at Iowa State University. Selected topics in Computational Learning Theory (PAC learning, Sample complexity, VC Dimension, Occam Learning, Boosting, active learning, Kolomogorov Complexity, Learning under helpful distributions, Mistake Bound Analysis). Selected topics in Bayesian and Information Theoretic Models (ML, MAP, MDL, MML). Advanced statistical methods for machine learning. Selected topics in reinforcement learning.
- Advanced Topics in Artificial Intelligence. Graduate course developed and taught at Iowa State University. Selected topics in federated learning, causal inference; deep learning; gaussian processes; longitudinal data analysis; representation learning; adversarial machine learning; semantic web; automated scientific discovery; neural and cognitive modeling.
- Artificial Intelligence Graduate Research Seminar Topics vary. Student-led discussion of research articles of current interest. Recent topics have included advanced topics in machine learning and knowledge representation. Offered every semester.
- Principles of Artificial Intelligence. Undergraduate course taught at Iowa State University. Specification, design, implementation, and selected applications of intelligent software agents and multi-agent systems. Computational models of intelligent behavior, including problem solving, knowledge representation, reasoning, planning, decision making, learning, perception, action, communication, and interaction. Reactive, deliberative, rational, adaptive, learning, and communicative agents. Artificial intelligence programming. Graduate credit requires a research

project and a written report. Oral and written reports.

• **Elements of Neural Computation**. Undergraduate course developed and taught at Iowa State University. Introduction to theory and applications of neural computation and computational neuroscience. Computational models of neurons and networks of neurons. Neural architectures for associative memory, knowledge representation, inference, pattern classification, function approximation, stochastic search, decision making, and behavior. Neural architectures and algorithms for learning including perceptions, support vector machines, kernel methods, learning, instance-based learning, reinforcement learning, unsupervised learning, and related techniques. Applications in Artificial Intelligence and cognitive and neural modeling. Hands-on experience is emphasized through simulation tools and laboratory projects. Oral and written reports.

DIVERSITY, EQUITY, and INCLUSION

I strongly believe that diversity of intellectual perspectives, gender, race, sexual identity and orientation, religious and cultural background, socioeconomic status, age, nationality, and methods of inquiry strengthens academic institutions, and contributes to excellence. This has driven me to work towards lowering the barriers faced by individuals coming from disadvantaged backgrounds in realizing their full potential as scientists, professionals, or scholars. Under my leadership, the NSF IGERT funded Bioinformatics and Computational Biology PhD program at ISU was able to attract and ensure the success of women and underrepresented minorities at rates significantly above the national average. In my role as a co-PI and executive committee member of the NSF-funded Northeast Big Data Hub, I worked with others on prioritizing the broadening of participation of underrepresented groups in data sciences, culminating in the establishment of the National Student Data Science Corps. I championed the creation of a core course in Responsible Data Science at Penn State. I have conducted research on algorithmic bias and fairness in machine learning and worked to incorporate discussions of it into the Data Sciences curriculum. I have worked to foster a diverse and welcoming environment in my laboratory and graduate and undergraduate programs that I have been involved in. I have regularly incorporated discussions of contributions of diverse individuals in computing and AI into the courses I teach. I am deeply committed to fostering inclusive excellence in all the programs that I have been part of.

CONSULTING

Scientific consulting on data mining, artificial intelligence, bioinformatics, semantic technologies, knowledge-based systems, information integration, and information technology for several corporations, startups, and government organizations.

OTHER PROFESSIONAL ACTIVITIES

(Not including memberships in editorships of journals and service on standing review panels and study sections e.g., NIH)

ADVISORY BOARDS AND WORKING GROUPS

- 2020- MDEpinet Taskforce on Blockchain and AI
- 2019- Ecosystem for Regional Networking (formerly Eastern Regional Network
- 2016 Transatlantic Data Science Workshop
- 2015-18 Electorate Nominating Committee, Information, Computing& Communication, AAAS
- 2016 IMA Workshop on Transdisciplinary Foundations of Data Science
- 2016- mProv, Data Provenance for Mobile Health Data MD2K Center, Univ. of Memphis
- 2015- Databrary, A Video Data Library for Developmental Science
- 2016- Posed2, Inc
- 2015- BioSNTR, an NSF EPSCOR Center at the University of South Dakota
- 2015-17 Chair, CCC Task Force on Convergence of Data and Computing
- 2016-17 CCC Task Force on Artificial Intelligence

CCC Task Force on Health IT 2014-16 2014 Masters Program in Data Science, Rochester Institute of Technology NSF INFEWS Workshop 2015 NSF Discovery Informatics Workshop 2012 NSF Knowledge Representation Workshop 2012 NSF Workshop on Population Health Measurement 2012 2012 NSF Workshop on Next Generation Financial Cyberinfrastructure 2011 mHealth Evidence Workshop, NIH Board of Directors, ACM Special Interest Group on Bioinformatics 2011-2012-13 Interagency Working Group on Multi-Scale Modeling IciS Workshop on Integrating, Representing, and Reasoning with Human 2010 Knowledge, Snowbird, Utah 2010 AFOSFR Workshop on Dynamic Data-Driven Application Systems, Arlington, VA 2005-External Advisory Committee, NSF HBCU-UP Program, Tuskegee University. Member of Advisory Board, Emergent Computational Neural Network 1999-03 Architectures, Universities of York, Edinburgh, and Sunderland, United Kingdom Member of Bioinformatics Group, National Science Foundation Intelligent Data 2004 Management PI Workshop, Boston, MA Member of Information Integration Working Group, National Science Foundation 2003 Intelligent Data Management PI Workshop, Seattle, WA. Member of Intelligent Agents Working Group, Information Institute, Information 1999 Directorate, Air Force Research Labs, Rome, New York 1999 Member of Search Committee, Senior Science and Technology Position in Defensive Information Warfare, Air Force Research Laboratory, Rome, New York. Proposal for a Ph.D. Program in Artificial Intelligence, University of Georgia Board 2000 of Regents Member, Intelligent Agents Working Group, Information Institute, Information 1999 Directorate, Air Force Research Labs Member, Intelligent Knowledge-Based Systems Working Group, Information 1998 Institute, Information Directorate, Air Force Research Labs Invited Participant, NSF Workshop on Decision Based Design, Sacramento, CA 1997

2025	Area Chair	AAAI Conference on Artificial Intelligence	
2024	Area Chair	AAAI Conference on Artificial Intelligence	
2023	Co-Chair	NSF Workshop on Machine Learning of Interatomic Potentials	
2022	Program Chair	AAAI Conference on Artificial Intelligence	
2022	Government Day	ACM SIGKDD Conference on Data Mining and Knowledge Discovery	
2021	Area Chair	AAAI Conference on Artificial Intelligence	
2020	Area Chair	AAAI Conference on Artificial Intelligence	
2019	Area Chair	AAAI Conference on Artificial Intelligence	
2018	Co-Chair	ACM SIGSOFT International Workshop on Automated Specification Inference	
2016	Chair	AAAI/CCC Workshop on Accelerating Science: A Grand Challenge for AI	

CONFERENCE OR WORKSHOP PROGRAM CHAIR

2015	Chair	PSB Workshop on Discovery Informatics	
2014	Co-chair	IEEE International Conference on Big Data	
2014	Program Co-Chair	IEEE Conference on Bio and Medical Informatics	
2014	Tutorial Program Chair	ACM Conference on Bioinformatics and Computational Biology	
2014	Co-chair	ACM SIGKDD Workshop on Discovery Informatics	
2014	Funding Co-chair	AAAI	
2013	Tutorial Program Chair	ACM Conference on Bioinformatics and Computational Biology	
2012	Workshop Program Chair	ACM Conference on Bioinformatics and Computational Biology	
2011	Co-Chair	ACM Immunoinformatics and Computational Immunology Workshop	
2011	Workshop Program Chair	ACM Conference on Bioinformatics and Computational Biology	
2011	Co-Chair	ACM Immunoinformatics & Comp. Immunology Workshop	
2010	Co-Chair	ACM Immunoinformatics & Comp. Immunology Workshop	
2010	Area Chair	IEEE Conference on Tools with Artificial Intelligence	
2009	Sponsorship co-chair	SIAM Conference on Data Mining	
2009	Area Chair	IEEE Conference on Tools with Artificial Intelligence	
2009	Organizer and Chair	Doctoral Student Forum, SIAM Conference on Data Mining	
2008	Vice Program Chair	International Semantic Web Conference	
2008	Track Chair	SIAM Conference on Data Mining	
2007	Organizer and Co- Chair	IJCAI Workshop on Semantic Web for Collaborative Knowledge Acquisition, IJCAI-2007 Hyderabad, India	
2006	Organizer and Co- Chair	First International Workshop on Modular Ontologies, International Semantic Web Conference, Athens, GA	
2006	Organizer and Co- Chair	AAAI Fall Symposium on Semantic Web for Collaborative Knowledge Acquisition (SweCKa 2006), Washington, DC.	
2005	Organizer and Chair	IEEE Workshop on Knowledge Acquisition from Distributed, Autonomous, Semantically Heterogeneous Information Sources, IEEE Conference on Data Mining, Houston, Texas	
2004	Program Co-Chair	International Conference on Intelligent Information Processing, Beijing, China	
2003	Organizer and Chair	Computational Intelligence Workshop John Vincent Atanasoff Symposium on Advanced Computing, Iowa State University, Ames, Iowa	
2002	Program Chair	Conference on Computational Biology and Genome Informatics, Durham, North Carolina	
2002	Track Chair	Artificial Life, Agents, and Adaptive Behavior Genetic and Evolutionary Computing Conference, New York	
2001	Organizer and Chair	Workshop on Knowledge Discovery from Heterogeneous, Distributed, Dynamic, Autonomous Data and Knowledge Sources. International Joint Conference on Artificial Intelligence Seattle.	
2001	Organizer and Co- Chair	Workshop on Cognitive Agents and Inter-agent Interaction, International Conference on Cognitive Science, Beijing	
2000	Organizer and Co- Chair	Workshop on Learning from Sequential and Temporal Data, International Conference on Machine Learning, Palo Alto, CA	

1999	Organizer and Co- Chair	Workshop on Computation with Neural Systems National Conference on Artificial Intelligence (AAAI), Orlando
1999	Track Chair	Artificial Life, Agents, and Adaptive Behavior Genetic and Evolutionary Computing Conference, Orlando
1998	Program Chair	International Colloquium on Grammatical Inference Ames, Iowa
1997	Organizer and Co- Chair	Workshop on Automata Induction, Grammatical Inference, and Language Acquisition International Conference on Machine Learning, Nashville
1992	Organizer and Chair	Workshop on Symbolic and Subsymbolic Information Processing, Neural Circuits and Systems, Conference on Neural Information Processing, Vail, CO

Conference Advisory Committee Membership

2008	Workshop on Web Service Composition and Adaptation, WSCA 2008
2007	Computational Structural Bioinformatics Workshop, BIBE 2007
2004	International Conference on Intelligent Knowledge Systems, Turkey
1997	International Conference on Evolutionary Computation
1997	International Conference on Artificial Intelligence, Cairo, Egypt

Conference or Workshop Program Committee Membership

2024	SPC, 27 th International Conference on Artificial Intelligence and Statistics (AISTATS-25)
2024	International Conference on Knowledge Discovery and Information Retrieval (KDIR-24)
2024	International Conference on Neural Computation Theory and Applications (NCTA-24)
2023	26 th International Conference on Artificial Intelligence and Statistics (AIStats-23)
2022	25 th International Conference on Artificial Intelligence and Statistics (AIStats-22)
2021	The AAAI-22 Workshop on Information-Theoretic Methods for Causal Inference and
	Discovery
2020	ACM/IMS Conference on the Foundations of Data Science
2019	PC Member, International Joint Conference on Artificial Intelligence
2018	PC Member, International Conference on Machine Learning
2017	SPC Member, AAAI Conference on Artificial Intelligence
2017	ACM Conference on Bioinformatics and Computational Biology
2016	AAAI Conference on Artificial Intelligence
2016	IEEE Conference on Bioinformatics and Biomedicine
2016	Conference on Data Integration in the Life Sciences
2016	ACM Conference on Bioinformatics and Computational Biology
2016	Data Science, Learning, and Applications to Biomedical & Health Sciences
2016	SPC Member, AAAI Conference on Artificial Intelligence
2015	PC Member, AAAI Conference on Artificial Intelligence
2015	PC Member, IEEE Conference on Bioinformatics and Biomedicine
2015	PC Member, Conference on Data Integration in the Life Sciences
2015	PC Member, ACM Conference on Bioinformatics and Computational Biology
2015	PC Member, AAAI Conference on Artificial Intelligence
2014	PC Member, AAAI Conference on Artificial Intelligence
2014	IEEE Big Data Congress
2014	ACM Conference on Bioinformatics, Computational Biology, and Health Informatics
2013	Conference on Data Integration in Life Sciences (DILS 2013)
2013	IEEE International Conference on Big Data

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2007	IEEE International Conference on Bioinformatics and Bioengineering (BIBE 2007)
2006	International Conference on Machine Learning (ICML 2006)
2006	AAAI Fall Symposium on Semantic Web for Collaborative Knowledge Acquisition (SweCKa 2006)
2006	First International Workshop on Modular Ontologies (WoMO 2006)
2006	IEEE Conference on Tools with Artificial Intelligence (ICTAI 2006)
2006	International Colloquium on Grammatical Inference (ICGI 2006)
2006	ACM / IEEE / WIC Conference on Web Intelligence (WI 2006)
2006	International Workshop on Algorithms in Bioinformatics (WABI 2006)
2006	8th International Conference on Data Warehousing and Knowledge Discovery
2006	IASTED International Conference on Computational Intelligence (CI 2006)
2006	IEEE Conference on Granular Computing (IEEE-GrC 2006)
2005	IEEE International Conference on Data Mining (ICDM 2005)
2005	International Conference on Algorithmic Learning Theory (ALT 2005)
2005	IEEE Conference on Tools with Artificial Intelligence (ICTAI 2005)
2005	International Conference on Machine Learning (ICML 2005)
2005	IEEE/ACM Conference on Intelligent Agent Technology (IAT 2005)
2005	ACM SIGKDD Workshop on Data Mining in Bioinformatics (BIOKDD 2005)
2005	Indian International Conference on Artificial Intelligence (IICAI 2005)
2004	IEEE International Conference on Data Mining (ICDM 2004)
2004	International Conference on Machine Learning (ICML 2004)
2004	IEEE/WIC/ACM Conference on Intelligent Agent Technology (IAT 2004)
2004	AAAI Workshop on Semantic Web Personalization
2004	IEEE Conference on Bioinformatics and Bioengineering (BIBE 2004)
2004	International Colloquium on Grammatical Inference (ICGI 2004)
2004	SIAM Bioinformatics Workshop, SIAM International Conference on Data Mining (SDM 04)
2004	IEEE Conference on Tools with Artificial Intelligence (ICTAI 2004)
2004	Midwestern Conference on Artificial Intelligence and Cognitive Science (MAICS 2004)
2003	IEEE International Conference on Data Mining (ICDM 2003)
2003	IEEE Conference on Tools with Artificial Intelligence (ICTAI 2003)
2003	International Conference on Intelligent Systems Design and Applications (ISDA 2003)
2003	Midwestern Conference on Artificial Intelligence and Cognitive Science (MAICS 2003)
2002	International Colloquium on Grammatical Inference (ICGI 2002)
2002	International Conference on Hybrid Intelligent Systems (HIS 2002)
2002	International Conference on Intelligent Systems Design and Applications (ISDA 2002)
2002	Midwestern Conference on Artificial Intelligence and Cognitive Science (MAICS 2002)
2002	Network Applications in Bioinformatics (NETTAB) Workshop at Bologna, Italy, 2002.
2002	Fourth International Workshop in Frontiers of Evolutionary Computation (FEA-2002)
2001	International Conference on Machine Learning (ICML 2001)
2001	International Symposium on Artificial Intelligence, India (ISAI 2001)
2001	International Joint Conference on Neural Networks (IJCNN 2001)
2001	International Conference on Hybrid Intelligent Systems (HIS 2001)
2001	SIAM Workshop on Mining Scientific Data Sets (at SDM 2001)
2001	Midwestern Conference on Artificial Intelligence and Cognitive Science (MAICS 2001)
2001	Genetic and Evolutionary Computing Conference (GECCO 2001)
2001	Workshop on Gene Expression. Genetic and Evolutionary Computing Conference, 2001
2000	International Colloquium on Grammatical Inference (ICGI 2000)

2000	Genetic and Evolutionary Computing Conference (GECCO 2000)
2000	Midwestern Conference on Artificial Intelligence and Cognitive Science (MAICS 2000)
1999	National Conference on Artificial Intelligence (AAAI 1999)
1999	Midwestern Conference on Artificial Intelligence and Cognitive Science (MAICS 1999)
1998	International Colloquium on Grammatical Inference (ICGI 1998)
1998	Genetic Programming Conference (GP 1998)
1997	International Conference on Machine Learning (ICML 1997)
1997	Genetic Programming Conference (GP 1997)
1996	Genetic Programming Conference (GP 1996)
1997	Midwest Artificial Intelligence and Cognitive Science Conference (MAICS 1997)
1996	World Congress on Neural Networks (WCNN 1996)
1996	Midwest Artificial Intelligence and Cognitive Science Conference (MAICS 1996)
1995	World Congress on Neural Networks (WCNN 1995)
1995	Midwest Artificial Intelligence and Cognitive Science Conference (MAICS 1995)
1993	International Simulation Technology Conference (SIMTEC 1993)
1993	University of New Brunswick Artificial Intelligence Symposium
1992	International Simulation Technology Conference (SIMTEC 1992)

Journal Referee

Applied Intelligence
Bioinformatics
BMC Bioinformatics
BMC Cancer
Connection Science
Genetic Programming
IEEE Computer
IEEE Expert
IEEE Intelligent Systems
IEEE Transactions on Data and Knowledge Engineering
IEEE Transactions on Evolutionary Computation
IEEE Transactions on Neural Networks
IEEE Transactions on Pattern Analysis and Machine Intelligence
IEEE Transactions on System, Man, and Cybernetics
International Journal of Data Mining and Bioinformatics
Information and Computation
Information Fusion
Information Sciences
Journal of Computational Biology
Journal of Machine Learning Research
Nucleic Acids Research
Neural Computation
Neural Networks
Machine Learning
Pattern Recognition
Proteins Structure, Function and Bioinformatics

Proposal Reviewer

National Science Foundation, USA
National Institutes of Health, USA
US Civilian Research Development Foundation, USA
United States Department of Agriculture, USA
Dutch National Science Foundation, Netherlands
European Physical Science and Engineering Research Council, United Kingdom
Irish National Science Foundation, Ireland
National Science and Engineering Research Council, Canada

Other Professional Service

Book and/or journal proposals for MIT Press, Academic Press, CRC Press, and Springer Verlag. External Referee, Promotion and Tenure.

DEPARTMENTAL, COLLEGE, AND UNIVERSITY SERVICE

	AL, COLLEGE, AND UNIVERSITY SERVICE	
2024-25	Member, Faculty Council, College of IST	PSU
2024-25	Member, Promotion and Tenure Committee, College of IST	PSU
2024-25	Member, Faculty Search Committee, AI for Climate Sciences	PSU
2023-24	Member, Inter-college Undergraduate AI Curriculum Committee	PSU
2023-24	Member, IST Dean Search Committee	PSU
2022-24	Member, Faculty Council, College of IST	PSU
2022-	Director, Center for AI Foundations and Scientific Applications	PSU
2023-24	Member, ICDS/HHD Faculty co-hire search committee	PSU
2023-24	Member, IST P&T Committee	PSU
2022-23	Member, Data Sciences Area P&T Committee, IST	PSU
2022-	Member, Faculty Council, College of IST	PSU
2022-23	Member, ICDS/IST AI Faculty co-hire search committee	PSU
2022-23	Member, ICDS/Animal Science Faculty Co-hire search committee	PSU
2022-23	Member, ICDS/Social Science Faculty Co-hire search committee	PSU
2021-22	Member, ICDS/IST AI Faculty Co-hire search Committee	PSU
2021-22	Member, ICDS/BME Data Science Faculty Co-hire Search Committee	PSU
2020-21	Member, ICDS/BME Data Science Faculty Co-hire Search Committee	PSU
2020-	Member AI Hub Coordination Committee, ICDS	PSU
2020-	Member, Data Sciences Coordination Committee	PSU
2015-	Director, Center for Big Data Analytics and Discovery Informatics	PSU
2014-	Associate Director, Institute for Computational and Data Sciences	PSU
2017-	Member, University Health Sciences Council	PSU
2019	AI in Medicine Symposium Organizer and Chair	PSU
2019-	Member, EHR research data governance committee	PSU
2019-	Member, Faculty Council, Institute for Computational and Data Sciences	PSU
2019-20	Member, Data Sciences Faculty Search Committee	PSU
2019-20	Member, Education and Data Science Faculty Search Committee	PSU
2018-19	Chair, Biomedical Data Sciences Faculty Search Committee	PSU
2018-19	Member, Astroinformatics Faculty Search Committee	PSU
2018-19	Member, Geoinformatics and Remote Sensing Faculty Search Committee	PSU
2017-20	Member, Faculty Council, College of IST	PSU
2018-19	Member, Informatics Graduate Program Advisory Committee	PSU
2018-	Member, Cognitive and Immersive Technologies Working Group	PSU
2016-17	Chair, Data Science faculty Search Committee, College of IST	PSU

2016-17	Faculty Council, College of IST		PSU
2016-17	Graduate Recruitment Committee		PSU
2016-	Executive Committee, Biomedical Data Sciences Training Program		PSU
2014-	Penn State Clinical and Translational Science	es Institute	PSU
2016-	Microbiome Center Executive Committee		PSU
2016-17	Promotion and Tenure Committee, College of IST		PSU
2016-	Data Sciences Program Supervisory Committee		PSU
2015-17	Research Advisory Committee, College of IS		PSU
2015-	Institute for Computational and Data Science		PSU
2015-16	Data Sciences Undergraduate Program Task		PSU
2016-	Research Data and Computing Committee, V		PSU
2015-16	Data Sciences Faculty Search Committee, Co	-	PSU
2014-16	Graduate Advisory Committee, College of IS	Т	PSU
2016-17	Lecturer Search Committee, College of IST		PSU
2015-17	Biomedical Engineering Search Committee		PSU
2013-14	Member, Vice Provost's Taskforce on Computing and Data Infrastructure		PSU
2013-14	Member, Strategic Planning Committee, College of Information Science and Technology		PSU
2005-2013	Director, Center for Computational Intelliger	nce, Learning and Discovery	ISU
2010-2011	Member, Supervisory Committee, Bioinformatics and Computational Biology Graduate Program		ISU
2009-2010	Director of Research	Computer Science	ISU
2009-2010	Director, Center for Computational Intelliger	nce, Learning and Discovery	ISU
2009-2010	Member, Research Computing Council		ISU
2009-2010	Chair, Promotion & Tenure Steering Committee	Computer Science	ISU
2009-2010	Member, Supervisory Committee, Bioinformatics and Computational Biology Undergraduate Program		ISU
2009-2010	Member, Supervisory Committee, Bioinformatics and Computational Biology Graduate Program		ISU
2009-2010	Director of Research	Computer Science	ISU
2008-2009	Member, Research Computing Council	•	ISU
2008-2009	Member, e-Science Steering Committee		ISU
2008-2009	Member, Promotion & Tenure Steering Committee	Computer Science	ISU
2008-2009	Member, Supervisory Committee, Bioinformatics and Computational Biology Undergraduate Program		ISU
2008-2009	Member, Supervisory Committee, Bioinformatics and Computational Biology Graduate Program		ISU
2007-2008	Member, Supervisory Committee, Bioinformatics and Computational Biology Undergraduate Program		ISU
2007-2008	Member, Research Computing Council		ISU
2007-2008	Member, Systems Biology Steering Committee		ISU
2007-2008	Member, Graduate Committee	Computer Science	ISU
2007-2008	Member, Promotion & Tenure Steering Committee	Computer Science	ISU
2007-2008	Member, Graduate Admissions Committee	Computer Science	ISU
	Member, Faculty Search Committee	Computer Science	ISU

2007-2008	Member, Professional and Scientific Staff Hiring Committee (ad hoc)	Computer Science	ISU
2007-2008	Director of Research	Computer Science	ISU
2006-2007	Member, Graduate Committee	Computer Science	ISU
2006-2007	Chair, Research Infrastructure Committee	Computer Science	ISU
2006-2007	Director of Research	Computer Science	ISU
2006-2007	Director, Center for Computational Intelligence, Learning and Discovery	ISU	ISU
2005-2006	Chair, Graduate Admissions Committee	Computer Science	ISU
2005-2006	Member, Departmental Web Committee	Computer Science	ISU
2005-2007	Ex Officio Member, Supervisory Committee, Bioinformatics & Computational Biology Graduate Program		ISU
2005-2007	Member, Planning Committee, Bioinformatics Undergraduate Program		ISU
2005-2006	Director of Research	Computer Science	ISU
2005-2006	Director, Center for Computational Intelligence, Learning and Discovery	ISU	ISU
2005-2006	Member, Promotion and Tenure Steering Committee	Computer Science	ISU
2004-2005	Member, Graduate Committee	Computer Science	ISU
2004-2005	Committee for review of the Office of the Vice President of Business & Finance		ISU
2003-2004	Member, ISU Information Technology Working	g Group: Research	ISU
2003-2004	Member, Graduate Admissions Committee	Computer Science	ISU
2002-2003	Member, Graduate Admissions Committee	Computer Science	ISU
2003-2004	Member, Provost's Information Technology Ac	lvisory Group	ISU
2002-2003	Member, Human Computer Interaction Graduate Program Steering Committee		ISU
2000-2001	Member, Department Chair Search Committee	Computer Science	ISU
1999-	Member, Supervisory Committee, Interdepartmental Bioinformatics & Computational Biology Graduate Program		ISU
1999	Coordinator, Complex Adaptive Systems Workshop		ISU
1999-2002	Member, Supervisory Committee, Complex Adaptive Systems Graduate Minor		ISU
1998-1999	Member, Graduate Committee	Computer Science	ISU
1998	Departmental Delegate, Annual Faculty Conference	Computer Science	ISU
1998	Member, Advisory Committee to Department Chair, Presidential Taskforce on Information Technology	Computer Science	ISU
1997-1998	Member, Graduate Committee	Computer Science	ISU
1996-1997	Member, Carver Trust Grant Proposal Review		ISU
1997-1999	Member, Bioinformatics & Computational Biology Program Steering Committee		ISU
1996-	Member, Promotion and Tenure Committee	Computer Science	ISU
1996-1997	Member, Graduate Committee	Computer Science	ISU
1996-1997	Coordinator, Graduate Student Orientation	Computer Science	ISU

1996	Member, Industry Day Organization Committee	Computer Science	ISU
1996	Advisor, Iowa State University Student Team,	AAAI Robot Competition	ISU
1996-1997	Member, Carver Trust Grant Proposal Review Committee		ISU
1995-1996	Faculty Secretary	Computer Science	ISU
1995-1999	Member, Interdepartmental Neuroscience Graduate Program Supervisory Committee		ISU
1994-1996	Member, Departmental Strategic Planning Committee	Computer Science	ISU
1990-1996	Member, Graduate Admissions Committee	Computer Science	ISU
1992-1994	Member, Liberal Arts and Sciences Honors Program Committee		ISU

References Available Upon Request