



PennState Institute for Computational and Data Sciences	Center for Artificial Intelligence Foundations & Scientific Applications Artificial Intelligence Research Laboratory	Q
What I do		
Machine learnin	g: Statistical, information theoretic, linguistic and structu	ural a

• Ma Iral approaches to machine learning; learning predictive relationships from sequential, graph-structured, multirelational, multimodal, partially specified, partially labeled, distributed data, linked data

PennState Clinical and Trans Science Institute

- · Causal Inference: Causal inference from disparate experimental and observational studies, causal inference from relational data, causal inference from temporal data
- Knowledge Representation and Inference: Logical, probabilistic, and decision-theoretic knowledge representation and inference; federated knowledge bases; selective information sharing; federated services; representing and reasoning about qualitative preferences
- Applied Informatics

- Bioinformatics: Prediction of macromolecular (protein-protein , protein-RNA, and protein-DNA) interaction networks, interfaces, and complexes; immune networks; microbiomes etc.
- Health Informatics: Predictive and causal modeling of health outcomes from patient (health records, genomics, socio-economic, environmental) data
- Brain Informatics: Modeling and analysis of structure and dynamics of brain networks
   Materials Informatics: Predicting material properties from structure and composition

#### Algorithmic Discovery

- Algorithmic abstractions of scientific domains
- Representations of scientific artifacts (experiments, data, models, assumptions, hypotheses, theories ...)
- Infrastructure for computationally mediated collaborative science

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Computation plays in many sciences a role that is analogous to played in transforming physics from a descriptive science (per predictive science (post Newton) • Computation is the sciences is calculus : Physics • Computation plays in many sciences a role that is analogous to played in transforming physics from a descriptive science (pre predictive science (post Newton) • Computation: Life sciences : : Calculus : Physics	ensitie de la constitute cience institute en science institute en synthetic en what calculus Newton) into a
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<ul> <li>Computation: Life sciences : : Calculus : Physics</li> </ul>	
<ul> <li>Computation: Social sciences : : Calculus : Physics</li> </ul>	
<ul> <li>Algorithms as theories: We understand a phenomenon when v algorithm that models it at the desired level of detail</li> </ul>	ve have an
Computing offers an exploratory apparatus for science: To the science is about acquiring, organizing, integrating, analyzing, a information, computing, science of information processing, pro apparatus for science	extent that nd reasoning with ovides exploratory
PennState Data Science for Researchers and Scholars	Vasant Honavar, Fall 2023





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Journ	ey from Philately to Physics	
• • • •	Brahe gathered 20 years of extremely accurat astronomical measurements: positions of the planets: data Kepler, working for Brahe, fit the data in ever imaginable to discover laws of planetary mot analytics and machine learning Newton and Leibnitz invented calculus – a lar expressing and reasoning about physical laws transforming natural philosophy into physics	te stars and y way ion: big data nguage for ; –
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PennState Comparison Artificial Intelligence Foundations & Scientific Applications Artificial Intelligence Research Laboratory	PennState Clinical and Translational Science Institute
Transformative potential of data science	
<ul> <li>Understanding physical, biological, cognitive, social and e systems – materials, cells, brains, individuals, organizatio</li> </ul>	engineered ns, societies
<ul> <li>Improving population health</li> </ul>	
<ul> <li>Anticipating and responding to crises</li> </ul>	
<ul> <li>Personalizing teaching and learning</li> </ul>	
<ul> <li>Defending critical infrastructure and services</li> </ul>	
<ul> <li>Making better decisions, e.g., public policy</li> </ul>	
<ul> <li>Making cities and communities smarter</li> </ul>	
<ul> <li>Improving food, energy, and water security</li> </ul>	
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# PennState Center for Artificial Intelligence Foundations & Scientific Applications PennState Instructer (computational and Data Science) Artificial Intelligence Research Laboratory Clinical and Transic Science Institute

# Data Science is a close cousin of Informatics



 Informatics is the study of the structure, behavior, and interactions of natural and engineered computational systems, including genomes, cells, brains, computers, organisms, societies.

- Data science shares the goal of understanding physical, biological, cognitive, social, and engineered systems
- Informatics is concerned with the representation, processing, and communication of information in such systems.
- Data science is concerned with formulating descriptive, predictive, and causal questions about the world around us and answering them using data

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The 12th pept Rate. Id the Reserved Re	1925 21	Budge Red Sex	83,592	> Centralt at HGP	
	1917 22	Reales Red Sea	\$3,500	7 Careford at HOF	83-W. \$5,000; Baaded Timping \$7,000
George Herman Ruth (Bobe, The Bambino or The Sulton Of Swat)	1925 23	Bestee Red Sec	\$9.800	7 Alar Week, 1958, at 383	Indules \$1,000 missesim rate, \$1,000 W5 tonus
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	1823 28	New York Farmers	\$12,000*	7 Richard Haupert research of eCP on	tracs B1 Janes Hearing Abland State 00.
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Final Games May 37, 1935 (App 40,213)	1828 23	New York Tankess	612,000*	7 Richard Haupert research of ROF on	etuca: 5/28/27 AL 46541 70000 AL
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	1997) Actor   Soundtrack   Greetor		Cast overview, first billed only: James Stewart		George Balley	
	James Haitland Stewart was born on 20 Ma	y 1906 in	Donna Reed		Mary Hatch	
	store. He was aducated at a local prep school, Mercersburg Academy, where he was a keen sthiete (football and		Uonel Barrymore		Mr. Potter	
	track), musician (singing and accordion pla sometime actor. In 1929 he won a place at where he studied See full bio +	ying), and Princeton,	Thomas Mitchell		Uncle Billy	
	Born: James Maitland Stewart May 20, 1908 in Indiana, Pennsylvania, USA		Henry Travers		Clarence	
	Died: July 2, 1997 (age 89) in Los Angeles USA	, California,	Beulah Bondi		Mrs. Balley	
		國國	Frank Faylen		Ernie	
		1 100	Ward Bond		Bert	
II 230 abetra 42 videos	1180 news articles a		Gioria Grahame		Violet	
Won 1 Oscar, Another 25 w	vins & 19 nominations. See more awards >		H.B. Warner		Mr. Gower	
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Data Science: Descriptive, Predictive, Causal
<ul> <li>Descriptive data science</li> <li>What is the gender distribution of STEM PhD recipients?</li> <li>How is gender correlated with income among physicians?</li> </ul>
<ul> <li>Predictive data science</li> <li>Can we predict degree completion based on student demographics, high school GPA, academic major?</li> <li>Can we predict voting preferences in presidential elections based on race, education, income, religious affiliation, marital status, and state of residence? If so, which variables are the most predictive of voting preferences?</li> </ul>
<ul> <li>Causal data science</li> <li>Does smoking cause cancer?</li> <li>How do diet and exercise modulate the risk of heart disease among those with a family history of heart disease?</li> </ul>
PennState Data Science for Researchers and Scholars Vasant Honavar, Fall 2023



### PennState Institute for Computational and Data Sciences

#### Center for Artificial Intelligence Foundations & Scientific Applications Artificial Intelligence Research Laboratory Clinical and Translat

## Course rationale

- Progress in many fields, including sciences and humanities, is increasingly enabled by our ability to acquire, share, integrate and analyze disparate types of data.
- Advances in data science methods and tools, coupled with large data sets, are leading to breakthroughs in many sciences.
- Consequently, there is a need for researchers, scholars, and practitioners, regardless of their disciplinary background and interests, to become proficient in applying modern data science methods and tools to gain useful insights from data.

e Data Science for

Scholars







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Learning outcomes	
Upon completion of this course, students should be ab	le to:
<ul> <li>Demonstrate broad understanding of the principles a data sciences</li> </ul>	and practice of
<ul> <li>Assess the feasibility of answering chosen research q available data and methods</li> </ul>	uestions using
<ul> <li>Choose the right method(s) in a given setting</li> </ul>	
Validate analyses	
<ul> <li>Ensure reproducibility of analyses</li> </ul>	
<ul> <li>Responsibly handle sensitive data</li> </ul>	
<ul> <li>Assess data and algorithmic bias</li> </ul>	
<ul> <li>Critically evaluate research and scholarly studies</li> </ul>	

 Effectively communicate the results of analyses to technical and non-technical audiences

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PennState Institute for Computational and Data Sciences	Illigence Foundations & Scientific Applications search Laboratory PennState Science Institute
Tentative outline	of topics
<ul> <li>What is data science?</li> <li>Mathematical preliminaries</li> <li>Python for Data Science</li> <li>Data Representation</li> <li>Descriptive statistics</li> <li>Exploratory Analysis: Clusterin</li> <li>Data Visualization</li> <li>Predictive Modeling</li> <li>Linear Algebra for Data Analys</li> <li>Probabilistic (generative) mod</li> <li>Evaluating predictive models</li> <li>Decision Trees</li> <li>Logistic Regression</li> <li>Multi-Class Extensions</li> </ul>	<ul> <li>Kernel Machines and Kernel Trick</li> <li>Kernel Machines: Kernel Design</li> <li>Ensemble Methods: Random Forests</li> <li>Deep Learning</li> <li>Representation Learning</li> <li>Responsible Data Science</li> <li>Analysis of Sensitive Data</li> <li>Important ideas in machine learning</li> <li>Causal Inference from data and assumptions</li> <li>Causal Inference from causal models</li> <li>Causal Inference using Machine Learning</li> <li>Review</li> </ul>

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## Center for Artificial Intelligence Foundations & Scientific Applications Artificial Intelligence Research Laboratory PennState Clinical and Transl Science Institute PennState **Course materials** Recommended Books Shah, Chirag (2020). A Hands-On Introduction to Data Science, Cambdridge University Press Skiena, S. (2017). Data Science Design Manual, Springer. Available for download by Penn State Students. • Behrman, K. (2022). Foundational Python for Data Science. • Watt, J., Borhani, R., Katsagellos, A. (2020). Machine Learning Refined. Cambridge University Press. Available through Penn State Libraries online. • Deisenroth, M.P., Faisal, A., and Ong, C.S. (2018) Math for Machine Learning. Cambridge University Press. Available through Penn State Libraries online. • Vanderplas, J. (2017). Python Data Science Handbook. O'Reilly. Freely available for online reading. · Lecture slides and readings to be posted on the study guide on the course web page https://faculty.ist.psu.edu/vhonavar/Courses/dsmethods/homepage.html Labs will be shared using google colab · Canvas will be used for everything else - announcements, course-related emails,

communicating with the instructor and the TA

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Grading							
<ul> <li>Lab Assignments: 30%</li> <li>Projects: 60%</li> <li>Class participation: 10</li> </ul>	<ul> <li>93% - 100% A</li> <li>90% - 93% A-</li> <li>87% - 90% B+</li> <li>83% - 87% B</li> <li>80% - 83% B-</li> <li>77% - 80% C+</li> <li>70% - 77% C</li> <li>60% - 70% D</li> <li>0% - 60% F</li> </ul>						

Please consult course policies regarding late assignments, and projects

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d Scholars

Vasant Honavar, Fall 2023

