Data Science Modules Enhancing the Biophysics Curriculum

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Statistics Online Computational Resource
Michigan Center for Applied & Interdisciplinary Mathematics
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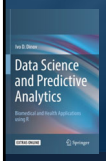
https://SOCR.umich.edu

Joint work with Magdalena Ivanova (Michigan)



STATISTICS ONLINE COMPUTATIONAL RESOURCE (SOCR)
UNIVERSITY OF MICHIGAN

Slides Online:
"SOCR News"

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Outline

- ❑ Motivation & Rationale
- ❑ Data Science Foundations

- ❑ Mathematical-physics, data science, artificial intelligence, and biomedical physics applications
- ❑ Data science and predictive analytics (DSPA) & biomedical physics with applications to disease (BPAD) R-based electronic markdown notebook

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Motivation & Rationale

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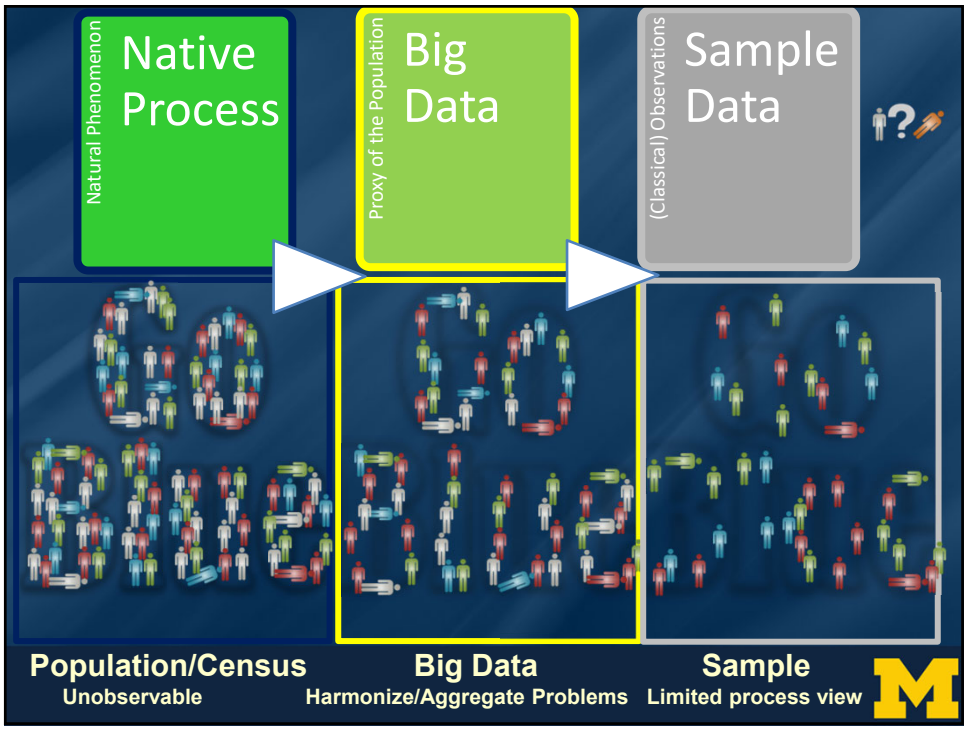

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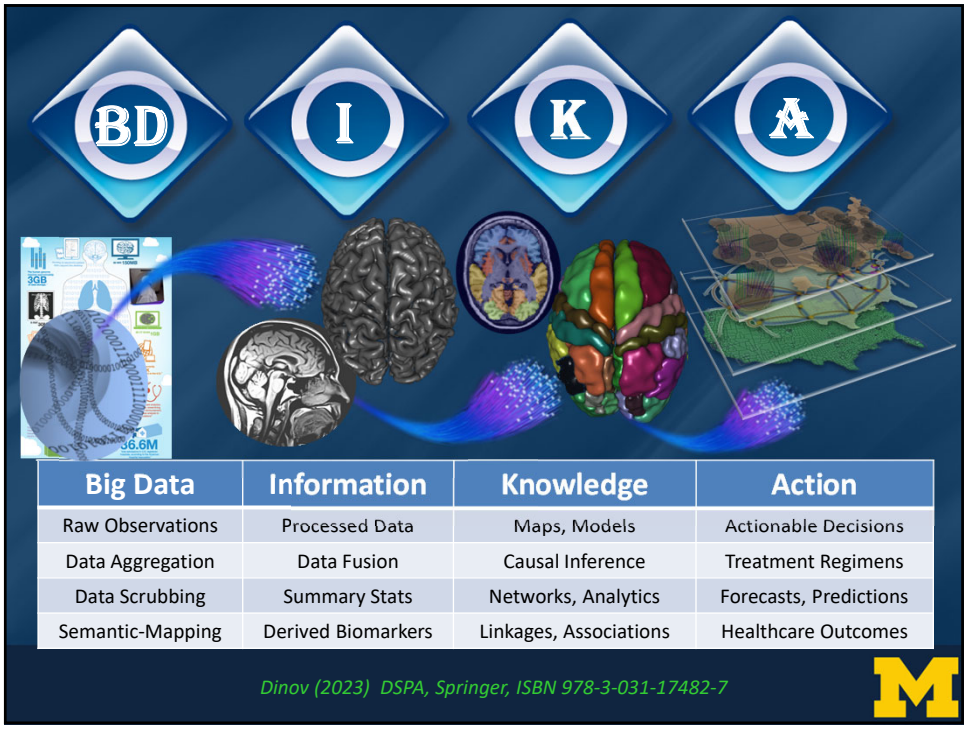

Big Data	Information	Knowledge	Action
Raw Observations	Processed Data	Maps, Models	Actionable Decisions
Data Aggregation	Data Fusion	Causal Inference	Treatment Regimens
Data Scrubbing	Summary Stats	Networks, Analytics	Forecasts, Predictions
Semantic-Mapping	Derived Biomarkers	Linkages, Associations	Healthcare Outcomes

Dinov (2023) DSPA, Springer, ISBN 978-3-031-17482-7

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Data Science Foundations

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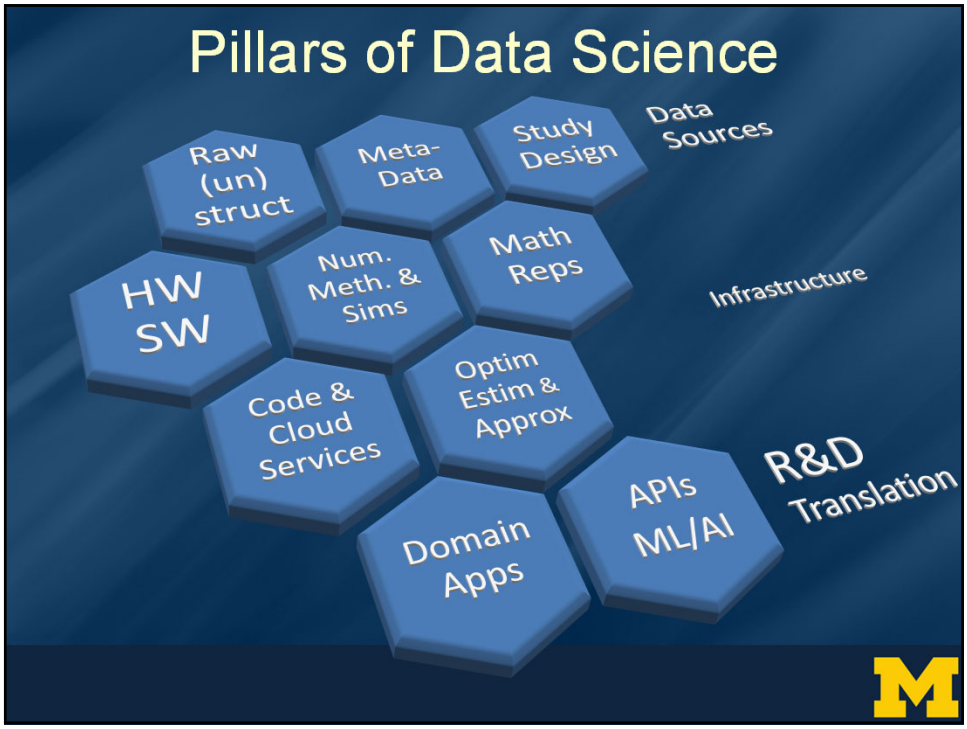

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Characteristics of Big Data

IBM Big Data 4V's: Volume, Variety, Velocity & Veracity

Big Bio Data Dimensions	Tools
Size	Harvesting and management of vast amounts of data
Complexity	Wranglers for dealing with heterogeneous data
Incongruency	Tools for data harmonization and aggregation
Multi-source	Transfer and joint modeling of disparate elements
Multi-scale	Macro to meso to micro scale observations
Time	Techniques accounting for longitudinal patterns in the data
Incomplete	Reliable management of missing data

Example: analyzing observational data of 1,000's Parkinson's disease patients based on 10,000's signature biomarkers derived from multi-source imaging, genetics, clinical, physiologic, phenomics and demographic data elements

Software developments, student training, service platforms and methodological advances associated with the Big Data Discovery Science all present existing opportunities for learners, educators, researchers, practitioners and policy makers

Dinov (2023) Springer

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Physics ↔ STEM ↔ Data Science R&D ↔ Education & Training Curricula

- ❑ Transdisciplinary training integrating *theoretical models, experimental science, computational algorithms, data science applications & domain-specific practice*
- ❑ Curriculum Models (*quant STEM-based* vs. *qual EDA-based*)
  - ❑ Lightweight (MOOCs, <12 semester credits),
  - ❑ Intermediate (13-29 credits)
  - ❑ Heavyweight (30-56 credits, UG/Grad) curricula
- ❑ Physics, Data Science and *X* Training Programs
- ❑ Some (Michigan) data science and biophysics course examples

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Spacekime Analytics: Example of Translating Mathematical-Physics ⟹ Data Science & AI

Physics	Data/Neuro Sciences
A **particle** is a small localized object that permits observations and characterization of its physical or chemical properties	An **object** is something that exists by itself, actually or potentially, concretely or abstractly, physically or incorporeal (e.g., person, subject, etc.)
An **observable** a dynamic variable about particles that can be measured	A **feature** is a dynamic variable or an attribute about an object that can be measured
Particle **state** is an observable particle characteristic (e.g., position, momentum)	**Datum** is an observed quantitative or qualitative value, an instantiation, of a feature
Particle **system** is a collection of independent particles and observable characteristics, in a closed system	**Problem**, aka Data System, is a collection of independent objects and features, without necessarily being associated with a priori hypotheses
Wave-function	**Inference-function**
Reference-Frame **transforms** (e.g., Lorentz)	Data **transformations** (e.g., wrangling, log-transform)
State of a system is an observed measurement of all particles ~ wavefunction	**Dataset (data)** is an observed instance of a set of datum elements about the problem system, $\boldsymbol{O} = \{\boldsymbol{X}, \boldsymbol{Y}\}$
A **particle system is computable** if (1) the entire system is logical, consistent, complete and (2) the unknown internal states of the system don't influence the computation (wavefunction, intervals, probabilities, etc.)	**Computable data object** is a very special representation of a dataset which allows direct application of computational processing, modeling, analytics, or inference based on the observed dataset
…	…

Dinov & Velev (2021)

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A Transdisciplinary Approach –
Biomedical Informatics & Data Science Training Program (BIDS-TP)

- **Fellows & Trainees**
  - BIDS Grads
  - BIDS Fellows (Seniors Yr 2)
  - New BIDS Fellows (Juniors Yr1)
  - BIDS Trainees (Junior and Senior)

- **Faculty Mentors** (~40)
- **Curriculum**: 18 credits: 4 core & 2 elective courses + other activities (seminars, workshops)
- **Outcomes Tracking**: Time to Degree, Completion Rate, Graduate Career Pathways, Trainees Awards & Fellowships, Publications (GoogleScholar & ORCID profiles), Soft Metrics
- **BIDS-TP Program Leadership**: Maureen Sartor, Margit Burmeister, Brian Athey, Ivo Dinov

https://bids-tp.umich.edu

Based on *Modernizing the Methods and Analytics Curricula for Health Science Doctoral Programs*
DOI: 10.3389/fpubh.2020.00022

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Medical Physics

- **BIOPHYS 430 / PHYSICS 430** (Traditional UG/Grad course), 3-credits, students from physics, chemistry, STEM, biosciences
- BPAD Mathematical Foundations »
  - Mathematical Foundations
  - Calculus of Differentiation and Integration
  - Scalars, Vectors, Matrices, and Tensors
  - Displacement, Velocity, and Acceleration
  - Polynomials, Exponents, and Logarithms
  - Taylor's Series Expansions
  - Complex Numbers
  - Ordinary Differential Equations
  - Probability and Statistics
    - Moments: Mean, Standard Deviation, Skewness, Kurtosis
    - Binomial Probability, Normal (Gaussian) & Poisson Probability Distributions
    - Joint Probability Distributions
    - Discrete and Continuous Variables (distributome.org)
  - Polar, Spherical and Cylindrical Coordinates
  - Partial Derivatives and PDEs
  - Linear Algebra (linear modeling is covered later in Chapter XII)
  - Dimensionality Reduction (PCA/ICA, t-SNE, UMAP)
  - https://socr.umich.edu/BPAD/BPAD_notes/Biophysics430_Chap01_MathFoundations.html

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Biophysics of Disease

- **BIOPHYS 440 / Chem 440** (Traditional UG/Grad course), 3-credits, students from physics, chemistry, STEM, bio sciences

- Kidney Imaging-Clinical Case Study
  - Overview
  - Meta-Data Import
    - Meta-Data Summaries
    - Suppress Boolean comorbidity columns
  - EDA
    - 1D Distributions (radiographic_size by surgery_type)
    - 2D+ Distributions (vital_days_after_surgery, surgical_approach)
  - Analytics
    - Logistic Regression - Predicting Patient Survival
  - Imaging data
    - Joint analysis of the clinical meta-data & volumetric imaging data

- https://socr.umich.edu/BPAD/BPAD_notes/Kidney_Imaging_Clinical_Dataset_2023.html

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Data Science & Predictive Analytics

- **HS650** (Traditional grad-level course + online self-guided MOOC), 4-credits, students from 6 colleges representing STEM, bio, econ, humanities

- Builds computational abilities, inferential thinking, and practical skills for tackling core data scientific challenges. Covers foundational concepts in data management, processing, statistical computing, and dynamic visualization using modern programming tools and agile web-services.
- Blends core math principles ad concepts with computational techniques, tools and services for managing, harmonizing, aggregating, preprocessing, modeling, analyzing and interpreting large, multi-source, incomplete, incongruent, and heterogeneous data (Big Data). Biomedical, healthcare, and social datasets provide context for addressing specific driving challenges.

Dinov, Springer (2023)

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Learning Resources & Instructional Materials

- EBooks
  - https://DSPA2.predictive.space
  - https://TCIU.predictive.space
  - https://BPAD.predictive.space
  - https://SpaceKime.org
- R Package
  - https://cran.rstudio.com/web/packages/TCIU
- GitHub
  - https://github.com/SOCR

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Demonstrations

- Distribution (model-based) inference
  https://doi.org/10.1007/s42979-022-01206-w & https://doi.org/10.52041/iase.pdsxt
  https://socr.umich.edu/HTML5/BivariateNormal/BVN2 & http://distributome.org/V3
  https://socr.umich.edu/HTML5/SOCRAT
- Apps
  Fourier/Wavelet: https://socr.umich.edu/HTML5/Fourier_Wavelet_app
  Large Tensors/UMAP/t-SNE: https://socr.umich.edu/HTML5/SOCR_TensorBoard_UKBB
  Morphogenesis: https://socr.umich.edu/BPAD/BPAD_notes/Biophysics430_Chap05_TransportInfiniteMedium.html
- DSPA (Rmarkdown eNotebook, R, Python, C, JS, …)
  https://socr.umich.edu/DSPA2/DSPA2_notes/05_SupervisedClassification.html#16_Case_Study:_Predicting_Galaxy_Spins
  https://socr.umich.edu/DSPA2/DSPA2_notes/10_SpecializedML_FormatsOptimization.html#17_R_Notebook_support_for_other_programming_languages
- Complex-time (Kime) & Spacekime Analytics
  https://www.socr.umich.edu/TCIU/HTMLs/Chapter4_TCIU_Predictive_Analytics.html
- SOCR & GitHub
  - https://socr.umich.edu & https://github.com/SOCR

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