Data Sharing – Open, Rigorous & Reproducible Science

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Outline

- Pillars of Open-Science
- Rationale (Pros & Cons)
- Big Data Sharing
- *DataSifter: Statistical obfuscation*
- Case-studies
  - ALS Study
  - Population Census-like Neuroscience (UKBB)
  - Spacekime Analytics

Pillars of Open-Science

Sources: Characteristics of Big Biomed Data

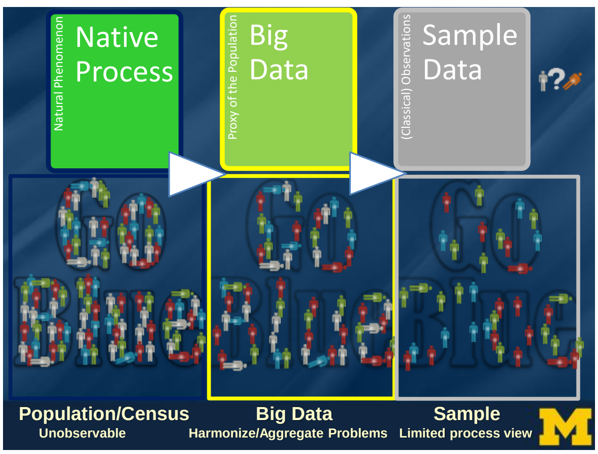
IBM Big Data 4V's: Volume, Variety, Velocity & Veracity

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 (2016) GigaScience   Dinov (2018) Springer



From 23 … to … 2^{23}

- Data Science: 1798 vs. 2020
- In the 18th century, Henry Cavendish used just 23 observations to answer a fundamental question – "What is the Mass of the Earth?" He estimated very accurately the mean density of the Earth/H_2O (5.483 ± 0.1904 g/cm^3)
- In the 21st century to achieve the same scientific impact, matching the reliability and the precision of the Cavendish's 18th century prediction, requires a monumental community effort using massive and complex information perhaps on the order of 2^{23} bytes
- Scalability and Compression
  (per Gerald Friedland/Berkeley): 23 ➔ $2^{23} \cong$ 10M

Cavendish (1798) Philosophical Transactions of the Royal Society of London | Dinov (2016) JSMI

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, et al. (2016) PMID:26918190

Why is FAIR Data Sharing Important?

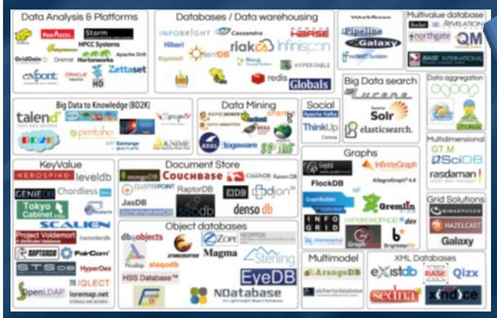
Data

- Optimum resource utilization (low cost, high efficiency / policy, security, processing complexity)
- Democratization of the scientific discovery process
- Enhanced inference (e.g., coverage of rare events, increase of stat power)
- Increase of Kryder's Law (Data volume) ≫ Moore's Law (Compute power)
- Exponential decay of data-value
- Incents innovation, transdisciplinary collaborations, and knowledge dissemination
- …

FAIR = Findable + Accessible + Interoperable + Reusable

Infrastructure: Cloud Ecosystem

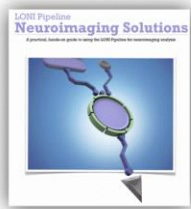
Cloud Services



https://socr.umich.edu/docs/BD2K/BigDataResourceome.html

Infrastructure: Cranium/Pipeline

Tools



http://Pipeline.loni.usc.edu

Dinov, et al. (2013) Brain Imaging and Behavior | Dinov, et al. (2014) Front. NeuroInfo.

Findings: OA Pubs/Sharing

Pubs

- OA Pubs
  - https://en.wikipedia.org/wiki/Open_access
  - https://arxiv.org | https://www.biorxiv.org
  - Blogs (e.g., https://TerryTao.wordpress.com)
- Cloud Services
  - Computing (e.g., Azure, Google, AWS)
  - Storage
  - ICT (information and communication technologies)
- SW
  - https://GitHub.com (e.g., https://github.com/SOCR)
  - http://Cran.r-project.org | Jupyter.org | Rmarkdown.rstudio.com
  - E.g., https://DSPA.predictive.space
- Licensing
  - https://www.gnu.org/licenses
  - https://socr.umich.edu/html/SOCR_CitingLicense.html

Findings: Open Science Career Assessment Matrix

Open Science activities	Metrics: Possible evaluation criteria
RESEARCH OUTPUT	
Research activity	Pushing forward the boundaries of open science as a research topic
Publications	Publishing in open access journals Self-archiving in open access repositories
Datasets and research results	Using the FAIR data principles Adopting quality standards in open data management and open datasets Making use of open data from other researchers
Open source	Using open source software and other open tools Developing new software and tools that are open to other users
Funding	Securing funding for open science activities
RESEARCH PROCESS	
Stakeholder engagement/ citizen science	Actively engaging society and research users in the research process Sharing provisional research results with stakeholders through open platforms (e.g. Arxiv, Figshare, OverLeaf) Involving stakeholders in peer review processes
Collaboration and Interdisciplinarity	Widening participation in research through open collaborative projects Engaging in team science through diverse cross-disciplinary teams
Research integrity	Being aware of the ethical and legal issues relating to data sharing, confidentiality, attribution and environmental impact of open science activities Fully recognizing the contribution of others in research projects, including collaborators, co-authors, citizens, open data providers
Risk management	Taking account of the risks involved in open science

Declaration on Research Assessment (DORA) | https://sfdora.org/good-practices/funders

Findings: Open Science Career Assessment Matrix

SERVICE & LEADERSHIP	
Leadership	Developing a vision and strategy on how to integrate OS practices in the normal research practice Driving policy and practice in open science Being a role model in practicing open science
Academic standing	Developing an international or national profile for open science activities Contributing as editor or advisor for open science journals or bodies
Peer review	Contributing to open peer review processes Examining or assessing open research
Networking	Participating in national and international networks relating to open science
RESEARCH IMPACT	
Communication and Dissemination	Participating in public engagement activities Sharing research results through non-academic dissemination channels Translating research into a language suitable for public understanding
IP (patents, licenses)	Knowledge on the legal and ethical issues relating to IPR Transferring IP to the wider economy
Societal impact	Evidence of use of research by societal groups Recognition from societal groups or for societal activities. **h-index, i10-index, sharing-index, other quant metrics of impact**
Knowledge exchange	Engaging in open innovation with partners beyond academia
TEACHING & SUPERVISION	
Teaching	Training other researchers in open science principles and methods Developing curricula and programs in open science methods, including open science data management Raising awareness and understanding in open science in undergraduate and masters' programs
Mentoring	Mentoring and encouraging others in developing their open science capabilities
Supervision	Supporting early stage researchers to adopt an open science approach
PROFESSIONAL EXPERIENCE	
Continuing professional development	Investing in own professional development to build open science capabilities
Project management	Successfully delivering open science projects involving diverse research teams
Personal qualities	Demonstrating the personal qualities to engage society and research users with open science Showing the flexibility and perseverance to respond to the challenges of conducting open science

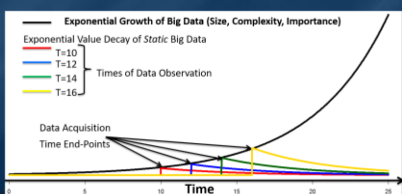
Declaration on Research Assessment (DORA) | https://sfdora.org/good-practices/funders

Rationale for Open Science (Cons)

- Journals impact factor (compared to pay-per-view journals, OA are newer)
- *Predatory* science (dubious quality, profit-centric, spam camouflage)
- Discovery is easy, but validity/utility of the science or tools may be difficult to evaluate *en masse*
- Extra work may be required by all scholars to sift through and identify appropriate materials
- Ambiguity of usage-rights/copyrights/licenses
- Democratization and socialization of science may suffer from some of the same downsides as social-networks
- Is science *competitive* or *collaborative*? Is it a *zero-sum* enterprise?

Rationale for Open Science (Pros)

- We are always stronger together
- Long-term sustainability prefers openness, inclusivity & diversity
- Optimized investments, career advancement, impact & cost-efficiency
- Expeditious discovery, innovation, productization & higher impact
- Rapid devaluation of data-hoarding, clandescent science, knowledge obfuscation
- …

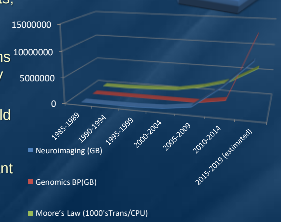


https://www.aaas.org/news/big-data-blog-part-v-interview-dr-ivo-dinov

Rationale for Open Science: Kryder vs. Moore

Collabs

- Moore's law = the expectation that our computational capabilities, specifically the number of transistors on integrated circuits, doubles approximately every 18-24 months.
- Kryder's law = the volume of data, in terms of disk storage capacity, is doubling every 14-18 months.
- **Kryder ≫ Moore**: Although both laws yield exponential growth, data volume is increasing at a faster pace. Thus, there are clear interests and needs for significant private, public and government engagement in opening, managing, processing, interrogating and interpreting the information content of Big Data.



Dinov (2016) SMSI | https://www.aaas.org/news/big-data-blog-part-v-interview-dr-ivo-dinov

Reliable, Effective & Secure Data Sharing

- Why is data-sharing difficult?
  monopoly, preservation of *status-quo,* competitive edge, personally identifiable information, IP protection, security (on multiple levels), red tape, …
- FAIR (Findable, Accessible, Interoperable & Reusable) Data are powerful
- Current Data Sharing Landscape?
  Differential Privacy, fully-homomorphic encryption, statistical obfuscation (DataSifter), …

DataSifter

- DataSifter is an iterative statistical computing approach that provides the data-governors controlled manipulation of the trade-off between sensitive information obfuscation and preservation of the joint distribution.
- The DataSifter is designed to satisfy data requests from pilot study investigators focused on specific target populations.
- Iteratively, the DataSifter stochastically identifies candidate entries, cases as well as features, and subsequently selects, nullifies, and imputes the chosen elements. This statistical-obfuscation process relies heavily on nonparametric multivariate imputation to preserve the information content of the complex data.

http://DataSifter.org US patent #16/051,881 Marino, *et al., JSCS* (2019)

DataSifter

- A detailed description and *dataSifter()* R method implementation are available on our GitHub repository (https://github.com/SOCR/DataSifter).
- Data-sifting different data archives requires customized parameter management. Five specific parameters mediate the balance between protection of sensitive information and signal energy preservation.

Obfuscation level	$0 \le \eta = \eta(k_0 + k_1 + k_2 + k_3 + k_4) \le 1$				
	k_0	k_1	k_2	k_3	k_4
None	0	0	0	0	**0**
Small	0	0.05	1	0.1	**0.01**
Medium	1	0.25	2	0.6	**0.05**
Large	1	0.4	5	0.8	**0.2**
Indep	Output synthetic data with independent features				

k_0: A Boolean; obfuscate the unstructured features?

k_1: proportion of artificial missing data values that should be introduced

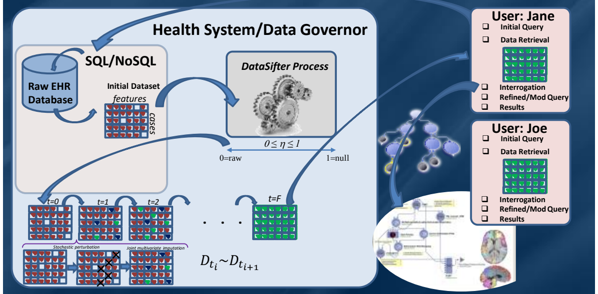
k_2: The number of times to iterate

k_3: The fraction of structured features to be obfuscated in all the cases

k_4: The fraction of closest subjects to be considered as neighbours of a given subject

http://DataSifter.org US patent #16/051,881 Marino, *et al.*, *JSCS* (2019)

DataSifter



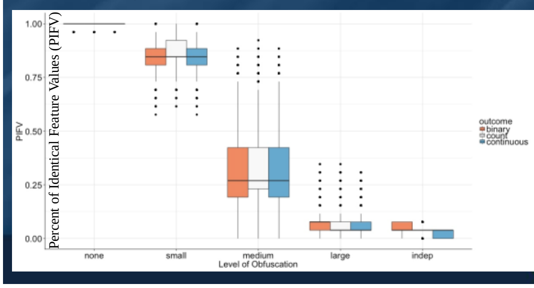
http://DataSifter.org US patent #16/051,881 Marino, *et al.*, *JSCS* (2019)

DataSifter Validation

I. Protection of sensitive information (privacy)

PIFV under Different Privacy Levels. Binary outcome refers to the first experiment; Count refers to the second experiment; Continuous refers to the third experiment.

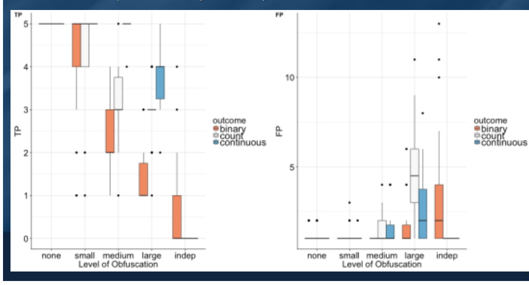
Each box represents 30 different "sifted" data or 30,000 "sifted" cases.



DataSifter Validation

II. Preserving utility information of the original dataset

Logistic Model with Elastic Net Signal Capturing Ability. TP is the number of true signals (total true predictors = 5) captured by the model. FP is the number of null signals that the model has falsely selected (total null signals=20).



DataSifter Validation

III. Clinical Data Application: Using DataSifter to Obfuscate the ABIDE Data

Comparing the Original and "Sifted" Data for the 22nd ABIDE Subject

η	Output	Sex	Age	Acquisition Plane	IQ	thick_std_ctx.lh.cuneus	curv_ind_ctx_lh_G_front_inf.Triangul	gaus_curv_ctx.lh.medialorbitofrontal	curv_ind_ctx_lh_S_interm_prim.Jensen
original	Autism	M	31.7	Sagittal	131	0.475	2.1	0.315	NA
none	Autism	M	31.7	Sagittal	131	0.475	2.1	0.315	0.51
small	Autism	M	31.7	Sagittal	131	0.475	2.1	0.315	0.4589
medium	Autism	M	31.7	Sagittal	111	0.548	2.85	0.315	0.463
large	Control	M	18.2	Sagittal	104	0.5347	3.198	0.1625	0.4524
indep	Control	M	15.4	Coronal	104	0.4842	3.383	0.1079	1.002

Autism Brain Imaging Data Exchange (ABIDE) case-study

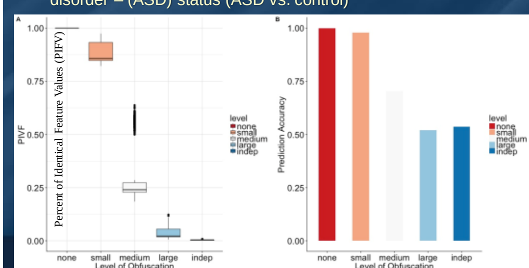
DataSifter Validation

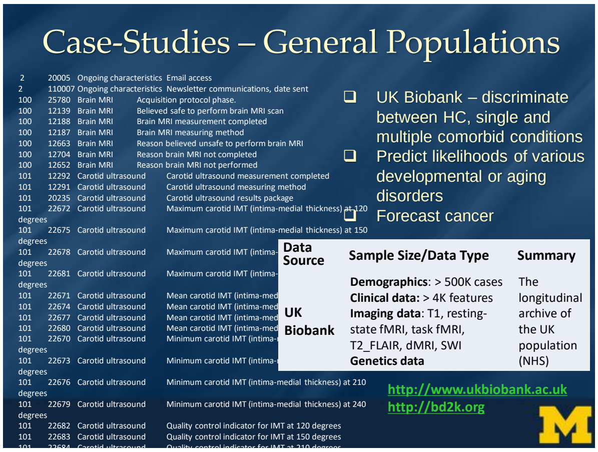
IV. Clinical Data Application: Using DataSifter to Obfuscate the ABIDE Data

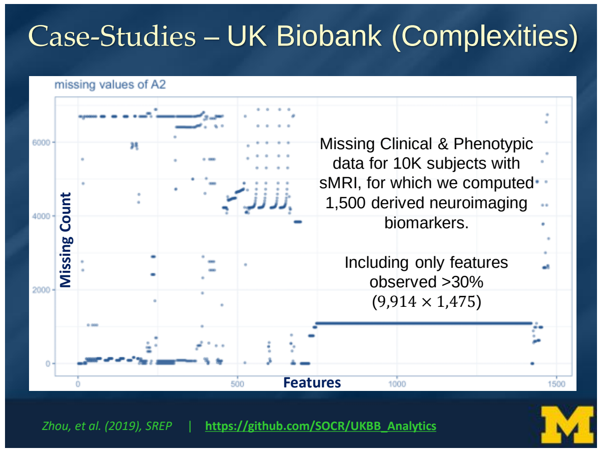
PIFVs for ABIDE under different levels of DataSifter obfuscations.

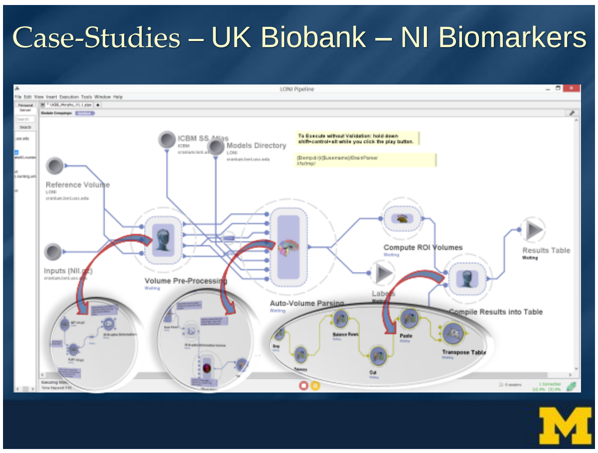
Each box represents 1098 subjects among the ABIDE sub-cohort

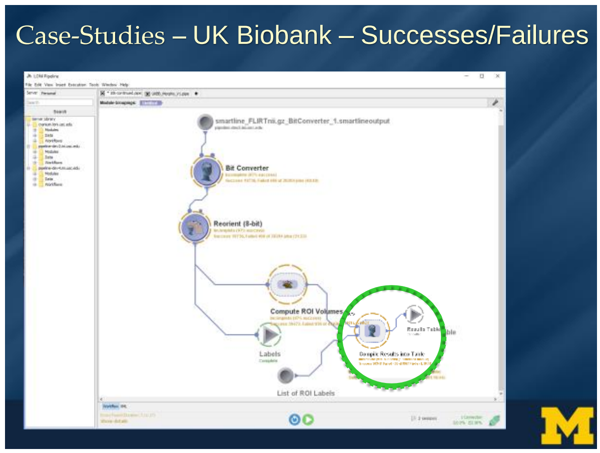
Random forest prediction of binary clinical outcome - autism spectrum disorder – (ASD) status (ASD vs. control)

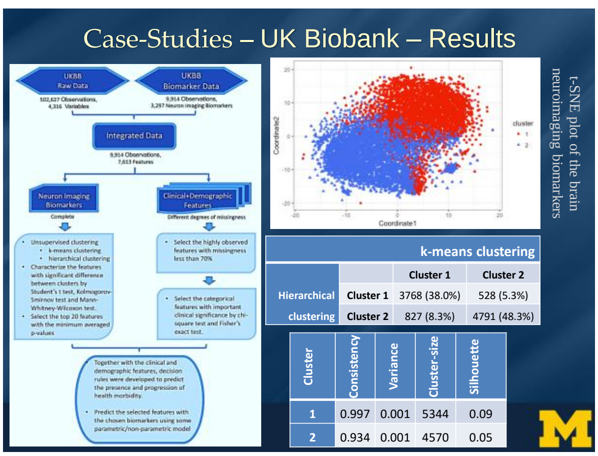


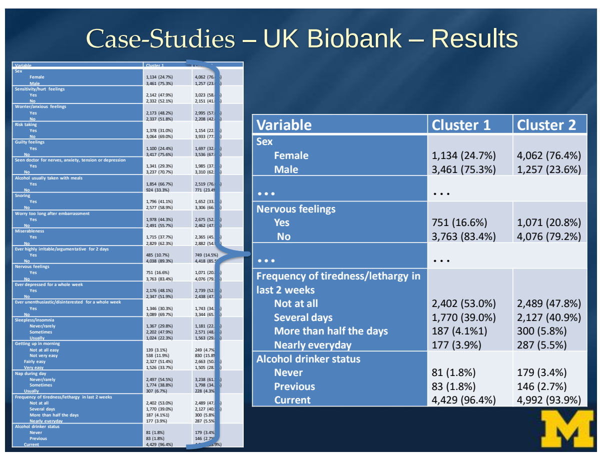

Case-Studies – General Populations
2 20005 Ongoing characteristics Email access
2 110007 Ongoing characteristics Newsletter communications, date sent
100 25780 Brain MRI Acquisition protocol phase.
100 12139 Brain MRI Believed safe to perform brain MRI scan
100 12188 Brain MRI Brain MRI measurement completed
100 12187 Brain MRI Brain MRI measuring method
100 12663 Brain MRI Reason believed unsafe to perform brain MRI
100 12704 Brain MRI Reason brain MRI not completed
100 12652 Brain MRI Reason brain MRI not performed
101 12292 Carotid ultrasound Carotid ultrasound measurement completed
101 12291 Carotid ultrasound Carotid ultrasound measuring method
101 20235 Carotid ultrasound Carotid ultrasound results package
101 22672 Carotid ultrasound Maximum carotid IMT (intima-medial thickness) at 120 degrees
101 22675 Carotid ultrasound Maximum carotid IMT (intima-medial thickness) at 150 degrees
101 22676 Carotid ultrasound Minimum carotid IMT (intima-medial thickness) at 210 degrees
101 22679 Carotid ultrasound Minimum carotid IMT (intima-medial thickness) at 240 degrees
101 22682 Carotid ultrasound Quality control indicator for IMT at 120 degrees
101 22683 Carotid ultrasound Quality control indicator for IMT at 150 degrees
UK Biobank – discriminate between HC, single and multiple comorbid conditions
Predict likelihoods of various developmental or aging disorders
Forecast cancer
Data Source
Sample Size/Data Type
Summary
UK Biobank
Demographics: > 500K cases
Clinical data: > 4K features
Imaging data: T1, resting-state fMRI, task fMRI, T2_FLAIR, dMRI, SWI
Genetics data
The longitudinal archive of the UK population (NHS)
http://www.ukbiobank.ac.uk
http://bd2k.org


Case-Studies – UK Biobank (Complexities)
missing values of A2
Missing Count
Features
Missing Clinical & Phenotypic data for 10K subjects with sMRI, for which we computed 1,500 derived neuroimaging biomarkers.
Including only features observed >30%
(9,914 × 1,475)
Zhou, et al. (2019), SREP | https://github.com/SOCR/UKBB_Analytics

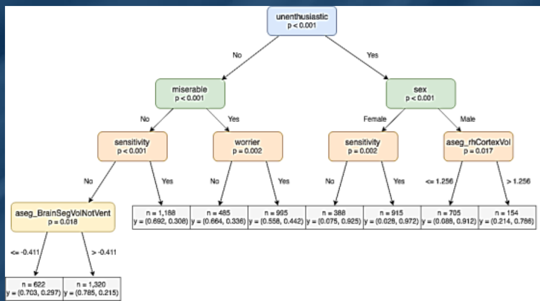

Case-Studies – UK Biobank – NI Biomarkers
Reference Volume
Inputs (NII.gz)
Volume Pre-Processing
Auto-Volume Parsing
Compute ROI Volumes
Results Table
Compile Results into Table
Transpose Table


Case-Studies – UK Biobank – Successes/Failures
Bit Converter
Reorient (8-bit)
Compute ROI Volumes
Labels
List of ROI Labels
Results Table


Case-Studies – UK Biobank – Results
UKBB Raw Data
502,627 Observations, 4,316 Variables
UKBB Biomarker Data
9,914 Observations, 3,297 Neuron Imaging Biomarkers
Integrated Data
9,914 Observations, 7,613 Features
Neuron Imaging Biomarkers
Complete
Clinical+Demographic Features
Different degrees of missingness
Unsupervised clustering
k-means clustering
hierarchical clustering
Characterize the features with significant difference between clusters by Student's t test, Kolmogorov-Smirnov test and Mann-Whitney-Wilcoxon test.
Select the top 20 features with the minimum averaged p-values
Select the highly observed features with missingness less than 70%
Select the categorical features with important clinical significance by chi-square test and Fisher's exact test.
Together with the clinical and demographic features, decision rules were developed to predict the presence and progression of health morbidity.
Predict the selected features with the chosen biomarkers using some parametric/non-parametric model
Coordinate1
Coordinate2
cluster
1
2
t-SNE plot of the brain neuroimaging biomarkers
k-means clustering
Cluster 1 | Cluster 2
Hierarchical clustering Cluster 1 | 3768 (38.0%) | 528 (5.3%)
Cluster 2 | 827 (8.3%) | 4791 (48.3%)
Cluster | Consistency | Variance | Cluster-size | Silhouette
1 | 0.997 | 0.001 | 5344 | 0.09
2 | 0.934 | 0.001 | 4570 | 0.05


Case-Studies – UK Biobank – Results
Variable | Cluster 1 | Cluster 2
Sex
Female | 1,134 (24.7%) | 4,062 (76.4%)
Male | 3,461 (75.3%) | 1,257 (23.6%)
• • • | • • •
Nervous feelings
Yes | 751 (16.6%) | 1,071 (20.8%)
No | 3,763 (83.4%) | 4,076 (79.2%)
• • • | • • •
Frequency of tiredness/lethargy in last 2 weeks
Not at all | 2,402 (53.0%) | 2,489 (47.8%)
Several days | 1,770 (39.0%) | 2,127 (40.9%)
More than half the days | 187 (4.1%1) | 300 (5.8%)
Nearly everyday | 177 (3.9%) | 287 (5.5%)
Alcohol drinker status
Never | 81 (1.8%) | 179 (3.4%)
Previous | 83 (1.8%) | 146 (2.7%)
Current | 4,429 (96.4%) | 4,992 (93.9%)

Case-Studies – UK Biobank – Results



Decision tree illustrating a simple clinical decision support system providing machine guidance for identifying **depression feelings** based on categorical variables and neuroimaging biomarkers. In each terminal node, the y vector includes the percentage of subjects being labeled as "no" and "yes", in this case, answering the question "Ever depressed for a whole week." The p-values listed at branching nodes indicate the significance of the corresponding splitting criterion.

Case-Studies – UK Biobank – Results

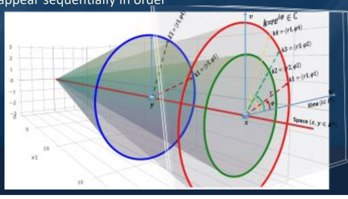
	Accuracy	95% CI (Accuracy)	Sensitivity	Specificity
Sensitivity/hurt feelings	0.700	(0.676, 0.724)	0.657	0.740
Ever depressed for a whole week	0.782	(0.760, 0.803)	0.938	0.618
Worrier/anxious feelings	0.730	(0.706, 0.753)	0.721	0.739
Miserableness	0.739	(0.715, 0.762)	0.863	0.548

Cross-validated (random forest) prediction results for four types of mental disorders

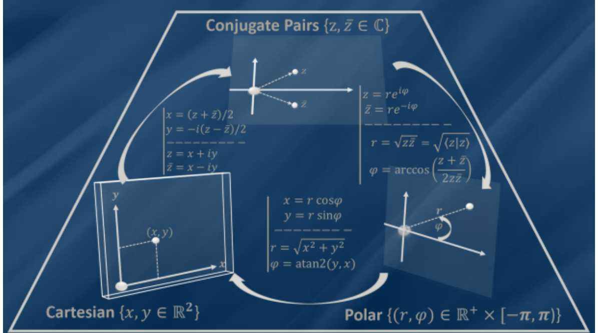
Zhou, et al. (2019), SREP

Complex-Time (*Kime*)

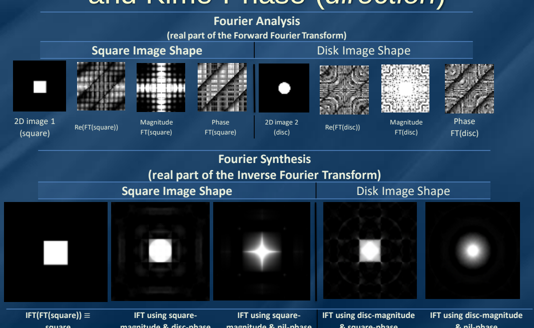
- At a given spatial location, $\boldsymbol{x}$, complex time (*kime*) is defined by $\kappa = re^{i\varphi} \in \mathbb{C}$, where:
  - the magnitude represents the longitudinal events order ($r > 0$) and characterizes the longitudinal displacement in time, and
  - event phase ($-\pi \le \varphi < \pi$) is an angular displacement, or event direction
- There are multiple alternative parametrizations of kime in the complex plane
- Space-kime manifold is $R^3 \times \mathbb{C}$:
  - $(\boldsymbol{x}, k1)$ and $(\boldsymbol{x}, k4)$ have the same spacetime representation, but different spacekime coordinates,
  - $(\boldsymbol{x}, k1)$ and $(\boldsymbol{y}, k1)$ share the same kime, but represent different spatial locations,
  - $(\boldsymbol{x}, k2)$ and $(\boldsymbol{x}, k3)$ have the same spatial-locations and kime-directions, but appear sequentially in order



Kime Parameterizations

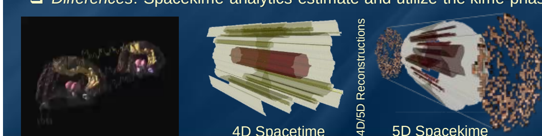


The Importance of Kime-Magnitude (*time*) and Kime-Phase (*direction*)



Longitudinal Data Analytics

- **Neuroimaging**:
  - *4D fMRI*: time-series, represents measurements of hydrogen atom densities over a 3D lattice of spatial locations ($1 \le x, y, z \le 64$ pixels), about 3×3 millimeters² resolution. Data is recorded longitudinally over time ($1 \le t \le 180$) in increments of about 3 seconds, then post-processed
  - *State-of-the-art Approaches*: Time-series modeling or Network analysis
  - *Spacekime Analytics*: 5D fMRI kime-series, represent the hydrogen atom densities over the same 3D lattice of spatial locations, longitudinally over the 2D kime space, $\kappa = re^{i\varphi} \in \mathbb{C}$
  - *Differences*: Spacekime analytics estimate and utilize the kime-phases



Dinov & Velev (2021)

Spacekime Calculus

❑ Kime **Wirtinger derivative** (first order kime-derivative at $\boldsymbol{k} = (r, \varphi)$):

In Cartesian coordinates:

$$f'(z) = \frac{\partial f(z)}{\partial z} = \frac{1}{2}\left(\frac{\partial f}{\partial x} - i\frac{\partial f}{\partial y}\right) \quad \text{and } f'(\bar{z}) = \frac{\partial f(\bar{z})}{\partial \bar{z}} = \frac{1}{2}\left(\frac{\partial f}{\partial x} + i\frac{\partial f}{\partial y}\right).$$

In Conjugate-pair basis: $df = \partial f + \bar{\partial} f = \frac{\partial f}{\partial z}dz + \frac{\partial f}{\partial \bar{z}}d\bar{z}.$

In Polar kime coordinates:

$$f'(k) = \frac{\partial f(k)}{\partial k} = \frac{1}{2}\left(\cos\varphi\frac{\partial f}{\partial r} - \frac{1}{r}\sin\varphi\frac{\partial f}{\partial \varphi} - i\left(\sin\varphi\frac{\partial f}{\partial r} + \frac{1}{r}\cos\varphi\frac{\partial f}{\partial \varphi}\right)\right) = \frac{e^{-i\varphi}}{2}\left(\frac{\partial f}{\partial r} - \frac{i}{r}\frac{\partial f}{\partial \varphi}\right)$$

$$f'(\bar{k}) = \frac{\partial f(\bar{k})}{\partial \bar{k}} = \frac{1}{2}\left(\cos\varphi\frac{\partial f}{\partial r} - \frac{1}{r}\sin\varphi\frac{\partial f}{\partial \varphi} + i\left(\sin\varphi\frac{\partial f}{\partial r} + \frac{1}{r}\cos\varphi\frac{\partial f}{\partial \varphi}\right)\right) = \frac{e^{i\varphi}}{2}\left(\frac{\partial f}{\partial r} + \frac{i}{r}\frac{\partial f}{\partial \varphi}\right).$$

❑ Kime **Wirtinger integration**:

Path-integral $\lim_{|z_{i+1}-z_i|\to 0} \sum_{i=1}^{n-1}\left(f(z_i)(z_{i+1}-z_i)\right) \cong \oint_{z_a}^{z_b} f(z_i)dz\,.$

Definite area integral: for $\Omega \subseteq \mathbb{C}$, $\int_\Omega f(z)dzd\bar{z}\,.$

Indefinite integral: $\int f(z)dzd\bar{z},\ df = \frac{\partial f}{\partial z}dz + \frac{\partial f}{\partial \bar{z}}d\bar{z}\,.$

The *Laplacian* in terms of conjugate pair coordinates is $\Delta f = d^2 f = 4\frac{\partial f}{dz}\frac{\partial f}{d\bar{z}} = 4\frac{\partial f}{d\bar{z}}\frac{\partial f}{dz}.$

Dinov & Velev (2021)

Quantum Mechanics, AI & Data Science

Mathematical-Physics	Data Science
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, $\boldsymbol{O} = \{X, Y\}$
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
…	…

Quantum Mechanics, AI & Data Science

Math-Physics	Data Science
Wavefunction Wave equ problem: $\left(\frac{\partial^2}{\partial x^2} - \frac{1}{\nu^2}\frac{\partial^2}{\partial t}\right)\psi(x,t) = 0$ Complex Solution: $\psi(x,t) = Ae^{i(kx-wt)}$ where $\left\lvert\frac{w}{k}\right\rvert = \nu$, represents a traveling wave	*Inference function* - describing a solution to a specific data analytic system (a problem). For example, • A linear (GLM) model represents a solution of a prediction inference problem, $\boldsymbol{Y} = \boldsymbol{X}\beta$, where the inference function quantifies the effects of all independent features ($\boldsymbol{X}$) on the dependent outcome ($\boldsymbol{Y}$), data: $\boldsymbol{O} = \{\boldsymbol{X}, \boldsymbol{Y}\}$: $\psi(\boldsymbol{O}) = \psi(X, Y) \ \Rightarrow\ \hat{\beta} = \hat{\beta}^{OLS} = \langle X\lvert X\rangle^{-1}\langle X\lvert Y\rangle = \left(X^T X\right)^{-1}X^T Y.$ • A non-parametric, non-linear, alternative inference is SVM classification. If $\boldsymbol{\psi_x} \in \boldsymbol{H}$, is the lifting function $\boldsymbol{\psi}: \boldsymbol{R^\eta} \to \boldsymbol{R^d}$ ($\boldsymbol{\psi}: \boldsymbol{x} \in \boldsymbol{R^\eta} \to \tilde{x} = \boldsymbol{\psi_x} \in \boldsymbol{H}$), where $\boldsymbol{\eta} \ll \boldsymbol{d}$, the kernel $\boldsymbol{\psi_x(y)} = \langle \boldsymbol{x}\lvert\boldsymbol{y}\rangle: \boldsymbol{O} \times \boldsymbol{O} \to \boldsymbol{R}$ transformes non-linear to linear separation, the observed data $\boldsymbol{O_i} = \{\boldsymbol{x_i}, \boldsymbol{y_i}\} \in \boldsymbol{R^\eta}$ are lifted to $\boldsymbol{\psi_{O_i}} \in \boldsymbol{H}$. Then, the SVM prediction operator is the weighted sum of the kernel functions at $\boldsymbol{\psi_{O_i}}$, where $\boldsymbol{\beta^*}$ is a solution to the SVM regularized optimization: $\langle\psi_O\lvert\,\beta^*\rangle_H = \sum_{i=1}^{n} p_i^* \langle\psi_O\lvert\psi_{O_i}\rangle_H$ The linear coefficients, $\boldsymbol{p_i^*}$, are the dual weights that are multiplied by the label corresponding to each training instance, $\{\boldsymbol{y_i}\}$. Inference always depends on the (input) data; however, it does not have 1-1 and onto bijective correspondence with the data, since the inference function quantifies predictions in a probabilistic sense.

GLM/SVM: https://DSPA.predictive.space | Dinov, Springer (2018)

Spacekime Analytics

❑ Let's assume that we have:
(1) Kime extension of Time, and
(2) Parallels between wavefunctions ↔ inference functions

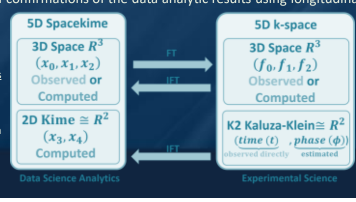
❑ Often, we can't directly observe (record) data natively in 5D spacekime.

❑ Yet, we can measure quite accurately the kime-magnitudes (r) as event orders, "times".

❑ To reconstruct the 2D spatial structure of kime, borrow tricks used by crystallographers [1] to resolve the structure of atomic particles by only observing the magnitudes of the diffraction pattern in k-space. This approach heavily relies on (1) prior information about the kime directional orientation (that may be obtained from using similar datasets and phase-aggregator analytical strategies), or (2) experimental reproducibility by repeated confirmations of the data analytic results using longitudinal datasets.

Spacetime → Spacekime Transforms

(1) Phase-estimation
(2) Phase-modeling
(3) Laplace Transform



[1] Rodriguez, Ivanova, Nature 2015

Spacekime Analytics: fMRI Example

❑ 3D isosurface Reconstruction of (2D space, 1D time) fMRI signal

4D spacetime: Reconstruction using trivial phase-angle; kime=time=(magnitude, 0)	**5D Spacekime**: Reconstruction using correct kime=(magnitude, phase)

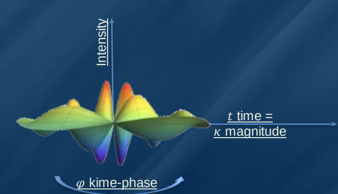
3D pseudo-spacetime reconstruction:

$$f = \hat{h}\,(\underbrace{x_1, x_2}_{space}, \underbrace{t}_{time})$$

Spacekime Analytics:
Kime-series = Surfaces (not curves)

In the 5D spacekime manifold, time-series curves extend to kime-series, i.e., surfaces parameterized by kime-magnitude (t) and the kime-phase (φ).

Kime-phase aggregating operators that can be used to transform standard time-series curves to spacekime kime-surfaces, which can be modeled, interpreted, and predicted using advanced spacekime analytics.



Bayesian Inference Representation

- We can formulate spacekime inference as a Bayesian parameter estimation problem:

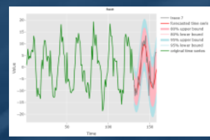
$$\underbrace{p(\gamma|X,\varphi')}_{\text{posterior distribution}} = \frac{p(\gamma,X,\varphi')}{p(X,\varphi')} = \frac{p(X|\gamma,\varphi')\times p(\gamma,\varphi')}{p(X,\varphi')} = \frac{p(X|\gamma,\varphi')\times p(\gamma,\varphi')}{p(X|\varphi')\times p(\varphi')} =$$
$$= \frac{p(X|\gamma,\varphi')}{p(X|\varphi')}\times\frac{p(\gamma,\varphi')}{p(\varphi')} = \frac{p(X|\gamma,\varphi')\times p(\gamma|\varphi')}{\underbrace{p(X|\varphi')}_{\text{observed evidence}}} \propto \underbrace{p(X|\gamma,\varphi')}_{\text{likelihood}} \times \underbrace{p(\gamma|\varphi')}_{\text{prior}}.$$

- In Bayesian terms, the posterior probability distribution of the unknown parameter γ is proportional to the product of the likelihood and the prior.
- In probability terms, the posterior = likelihood times prior, divided by the observed evidence, in this case, a single spacetime data point, x_{i_o}.

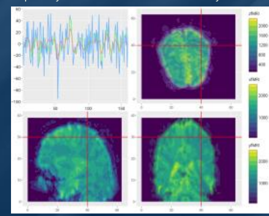
Spacekime Analytics using fMRI

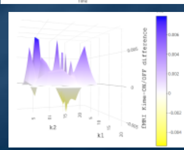
- Complex-valued *finger tapping* fMRI ($64x\ 64y\ 40z\ 160t$)

fMRI time-series forecasting

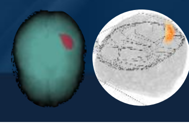


Temporal Dynamics of a Voxel in Somatosensory Motor Area





On-Off fMRI time-series to Kimesurface



What's Next?

- Lots of "open problems" in data-science, e.g., fundamentals of data representation & analytics
- The SOCR team is developing:
  - Compressive Big Data Analytics (CBDA) technique – an ensemble learning meta-algorithm
  - DS Time-Complexity and Inferential-Uncertainty
- Need lots of community, institutional, state, federal, and philanthropic support to advance open data science methods, enhance the computing infrastructure, train/support students/fellows, and tackle the *Kryder Law* $\gg$ *Moore Law* trend
- **Web**: https://SOCR.umich.edu
- **Git**: https://github.com/SOCR
- **Projects:** https://socr.umich.edu/html/SOCR_Research.html
- **Apps:** https://socr.umich.edu/HTML5/

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Acknowledgments

Slides Online: "SOCR News"

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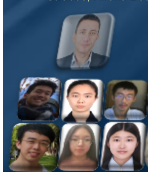

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