

## Big Neuroscience, Data Sharing & Predictive Health Analytics

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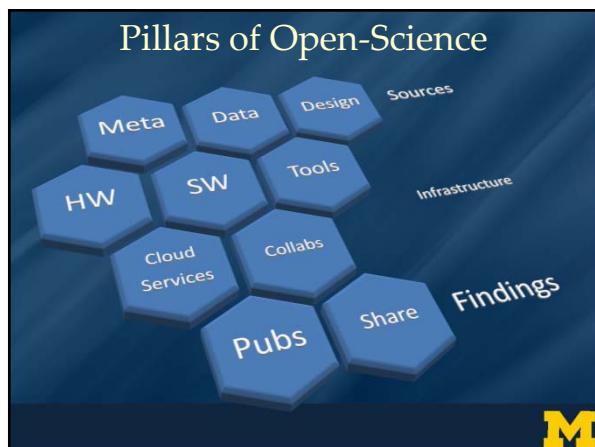
Slides Online: "SOCR News"

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## Outline

- ❑ Pillars of Open-Science
- ❑ Big Neuroscience
- ❑ Health Analytics
- ❑ *Data-Sharing via DataSifter Statistical Obfuscation*
- ❑ Case-studies
  - ❑ ALS Study
  - ❑ Population Census-like Neuroscience (UKBB)
  - ❑ Spacekime Analytics

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## Sources: Characteristics of Big Biomed Data

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

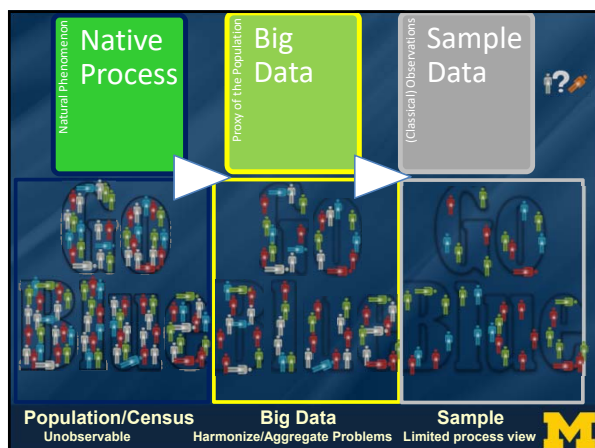
Big Bio Data Dimensions	Tools
Size	Harvesting and management of vast amounts of data
Complexity	Wranglers for dealing with heterogeneous data
Incongruency	Tools for data harmonization and aggregation
Multi-source	Transfer and joint modeling of disparate elements
Multi-scale	Macro to meso to micro scale 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

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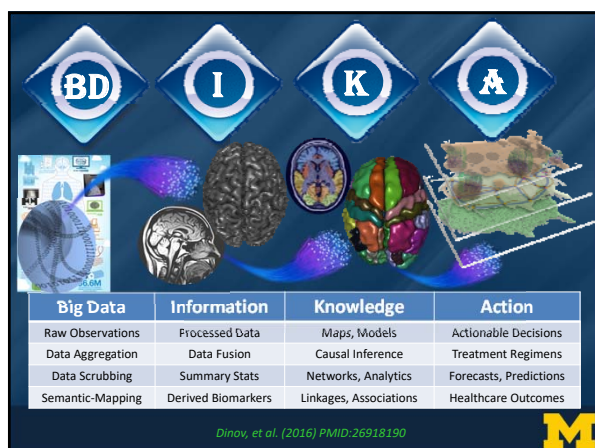


## From 23 ... to ... $2^{23}$

- ❑ Data Science: 1798 vs. 2019
- ❑ In the 18<sup>th</sup> 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<sub>2</sub>O ( $5.483 \pm 0.1904$  g/cm<sup>3</sup>)
- ❑ In the 21<sup>st</sup> century to achieve the same scientific impact, matching the reliability and the precision of the Cavendish's 18<sup>th</sup> 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):  $23 \rightarrow 10M$

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

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## Why is FAIR Data Sharing Important?

- ❑ 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 statistical power)
- ❑ Increase of Kryder's Law (Data volume) >> Moore's Law (Compute power)
- ❑ Exponential decay of data-value
- ❑ Incentivizes innovation, transdisciplinary collaborations, and knowledge dissemination
- ❑ ...

FAIR = Findable + Accessible + Interoperable + Reusable

## Infrastructure: Cloud Ecosystem



## Infrastructure: Cranium/Pipeline



## Findings: OA Pubs/Sharing

- ❑ OA Pubs
  - ❑ [https://en.wikipedia.org/wiki/Open\\_access](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>)
  - ❑ <https://Cran.r-project.org> | [Jupyter.org](https://jupyter.org) | [Rmarkdown.rstudio.com](https://Rmarkdown.rstudio.com)
  - ❑ E.g., <https://DSPA.predictive.space>
- ❑ Licensing
  - ❑ <https://www.gnu.org/licenses> (e.g., [http://socr.umich.edu/html/SOCR\\_CitingLicenses.html](http://socr.umich.edu/html/SOCR_CitingLicenses.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 Being aware of the ethical and legal issues relating to data sharing, confidentiality, attribution and environmental impact of open science activities
Research integrity	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://f1000.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://sfidora.org/good-practices/funders>



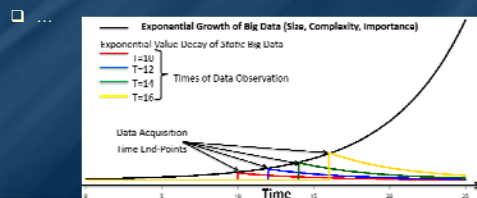
## Rationale for Open Science (Cons)

- ❑ 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 diversity
- ❑ Optimized investments, career advancement, impact & cost-efficiency
- ❑ Expeditious discovery, innovation, productization & impact
- ❑ Rapid devaluation of data-hoarding, clandestine science, knowledge obfuscation

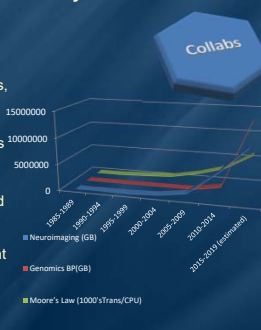


<https://www.aas.org/news/big-data-blog-part-v-interview-dr-ivo-dinov>



## Rationale for Open Science: Kryder vs. Moore

- ❑ **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.aas.org/news/big-data-blog-part-v-interview-dr-ivo-dinov>



## 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	$0 \leq \eta = \eta(k_0 + k_1 + k_2 + k_3 + k_4) \leq 1$				
	$k_0$	$k_1$	$k_2$	$k_3$	$k_4$
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				

$k_3$ : 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

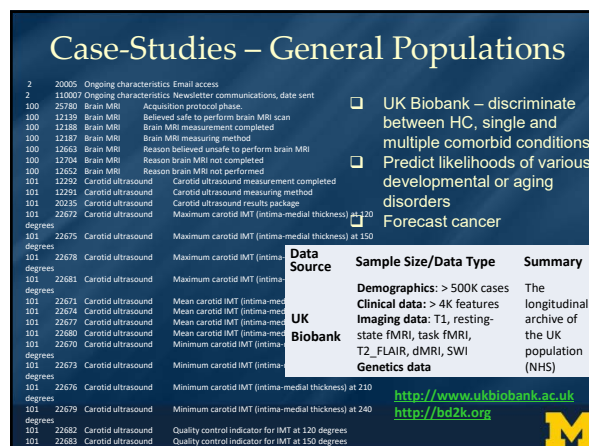
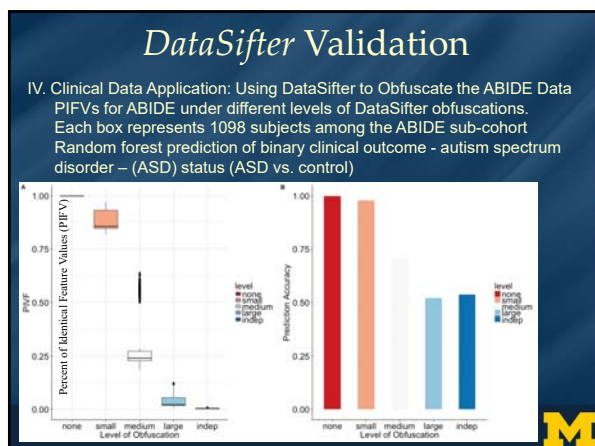
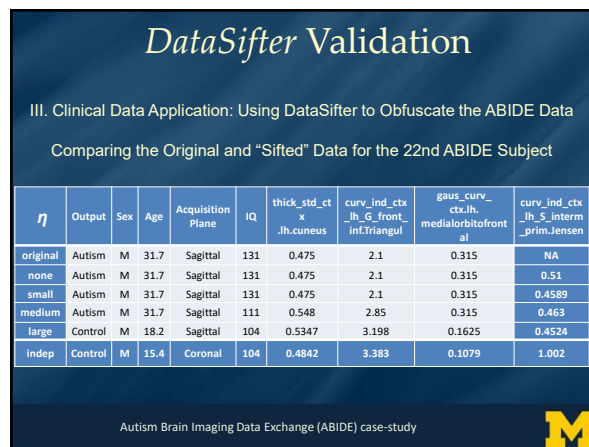
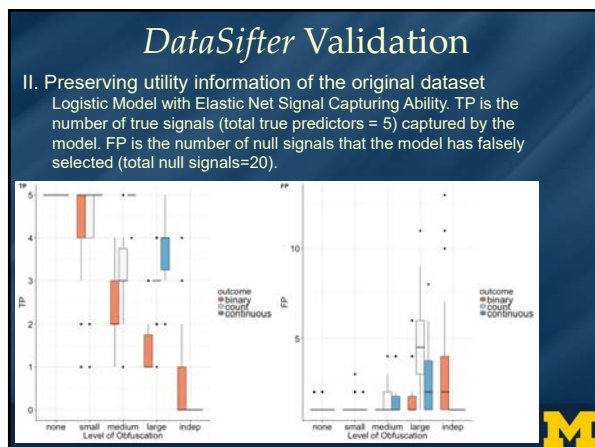
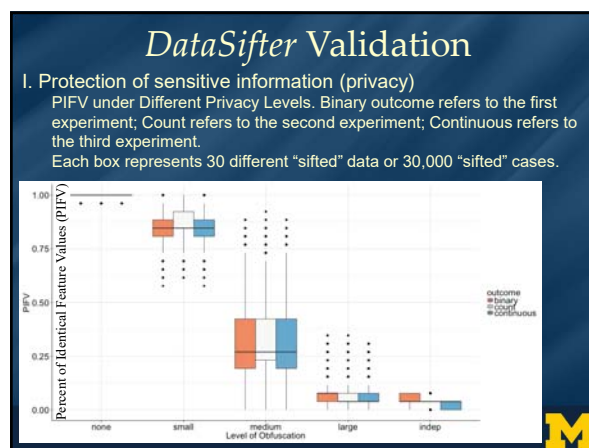
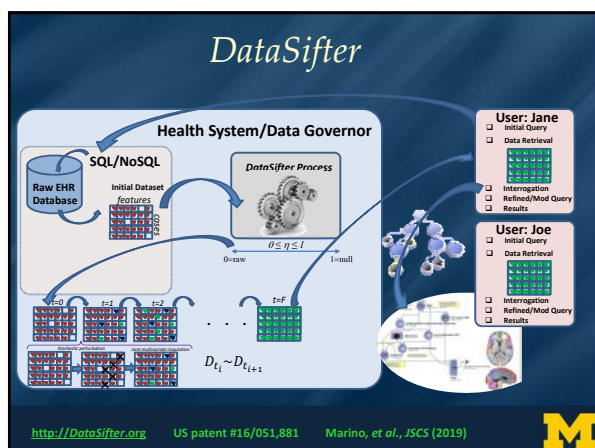
$k_3$ : The fraction of structured features to be obfuscated in all the cases

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

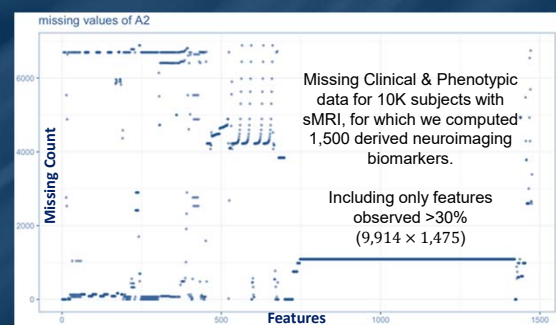
<http://DataSifter.org> US patent #16/051,881 Marino, et al., JSCS (2019)







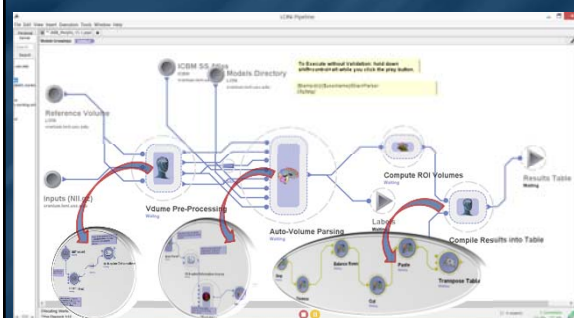
## Case-Studies – UK Biobank (Complexities)



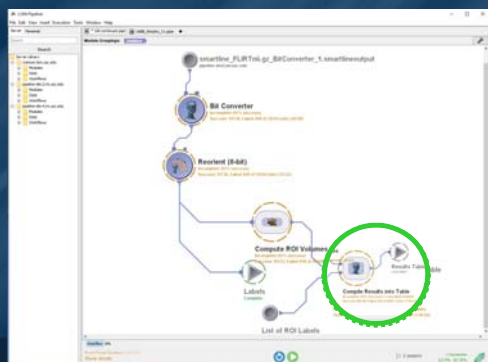
Zhou, et al. (2019), SREP | [https://github.com/SOCR/UKBB\\_Analytics](https://github.com/SOCR/UKBB_Analytics)



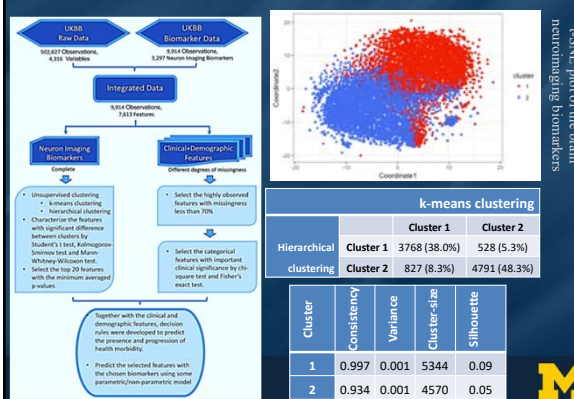
## Case-Studies – UK Biobank – NI Biomarkers



## Case-Studies – UK Biobank – Successes/Failures



## Case-Studies – UK Biobank – Results



t-SNE plot of the brain neuroimaging biomarkers

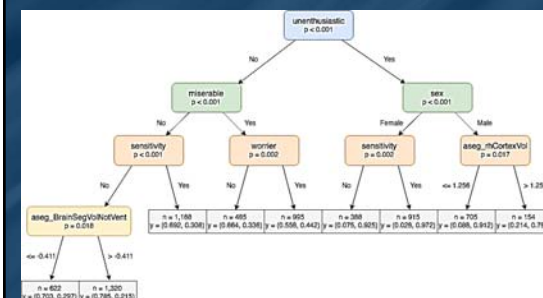


## Case-Studies – UK Biobank – Results

Variable	Cluster 1	Cluster 2
<b>Sex</b>		
Female	1,134 (24.7%)	4,062 (76.4%)
Male	3,461 (75.3%)	1,257 (23.6%)
***		
<b>Nervous feelings</b>		
Yes	751 (16.6%)	1,071 (20.8%)
No	3,763 (83.4%)	4,076 (79.2%)
***		
<b>Frequency of tiredness/lethargy in last 2 weeks</b>		
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%)	300 (5.8%)
Nearly everyday	177 (3.9%)	287 (5.5%)
<b>Alcohol drinker status</b>		
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

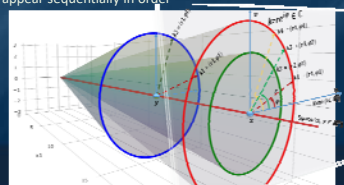
	Accuracy	95% CI (Accuracy)	Sensitivity	Specificity
Sensitivity/hurt feelings	0.700	(0.676, 0.724)	0.657	0.740
Ever depressed for a whole week	0.782	(0.760, 0.803)	0.938	0.618
Worrier/anxious feelings	0.730	(0.706, 0.753)	0.721	0.739
Miserableness	0.739	(0.715, 0.762)	0.863	0.548

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

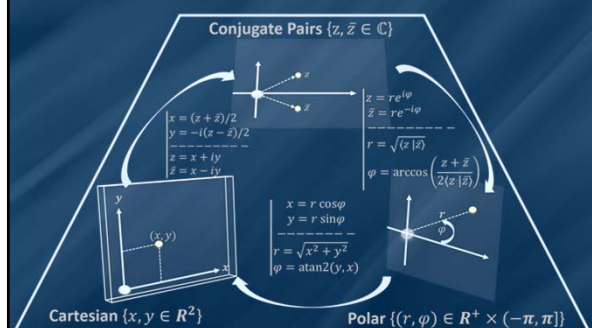
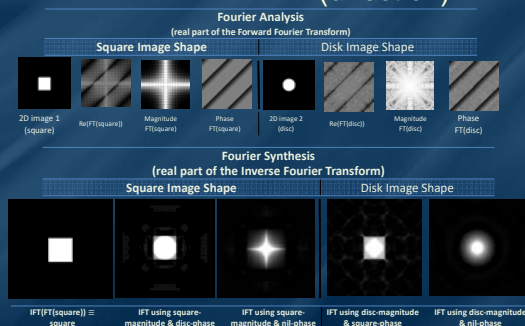
Zhou, et al. (2019), SREP

Complex-Time (*Kime*)

- At a given spatial location,  $x$ , 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 ( $-\pi \leq \varphi < \pi$ ) is an angular displacement, or event direction
- There are multiple alternative parametrizations of kime in the complex plane
- Space-kime manifold is  $R^3 \times \mathbb{C}$ :
  - $(x, k1)$  and  $(x, k4)$  have the same spacetime representation, but different spacekime coordinates,
  - $(x, k1)$  and  $(y, k1)$  share the same kime, but represent different spatial locations,
  - $(x, k2)$  and  $(x, k3)$  have the same spatial-locations and kime-directions, but appear sequentially in order



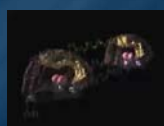
## Kime Parameterizations

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 ( $1 \leq x, y, z \leq 64$  pixels), about  $3 \times 3$  millimeters<sup>2</sup> resolution. Data is recorded longitudinally over time ( $1 \leq t \leq 180$ ) 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  $k = (r, \varphi)$ ):

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

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

In Polar kime coordinates:

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

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

- Kime **Wirtinger integration**:

$$\text{Path-integral} \quad \lim_{|z_{i+1}-z_i| \rightarrow 0} \sum_{i=1}^{n-1} (f(z_i)(z_{i+1} - z_i)) \cong \oint_{\gamma} f(z) dz.$$

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

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

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

Dinov & Velev (2021)





## Quantum Mechanics, AI & Data Science

### Mathematical-Physics

A **particle** is a small localized object that permits observations and characterization of its physical or chemical properties

An **observable** is a dynamic variable about particles that can be measured

Particle **state** is an observable particle characteristic (e.g., position, momentum)

Particle **system** is a collection of independent particles and observable characteristics, in a closed system

#### Wave-function

Reference-Frame **transforms** (e.g., Lorentz)

**State of a system** is an observed measurement of all particles ~ wavefunction

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.)

### Data Science

An **object** is something that exists by itself, actually or potentially, concretely or abstractly, physically or incorporeal (e.g., person, subject, etc.)

A **feature** is a dynamic variable or an attribute about an object that can be measured

**Datum** is an observed quantitative or qualitative value, an instantiation, of a feature

**Problem**, aka Data System, is a collection of independent objects and features, without necessarily being associated with a priori hypotheses

#### Inference-function

Data **transformations** (e.g., wrangling, log-transform)

**Dataset (data)** is an observed instance of a set of datum elements about the problem system,  $O = \{X, Y\}$

**Computable data object** is a very special representation of a dataset which allows direct application of computational processing, modelling, analytics, or inference based on the observed dataset

## Quantum Mechanics, AI & Data Science

### Math-Physics

#### Wavefunction

Wave equ problem:

$$\left(\frac{\partial^2}{\partial x^2} - \frac{1}{v^2} \frac{\partial^2}{\partial t^2}\right) \psi(x, t) = 0$$

Complex Solution:

$$\psi(x, t) = A e^{i(kx - \omega t)}$$

where  $\frac{|\omega|}{|k|} = v$ ,

represents a traveling wave

### Data Science

**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,  $Y = X\beta$ , where the inference function quantifies the effects of all independent features ( $X$ ) on the dependent outcome ( $Y$ ), data,  $O = \{X, Y\}$ :

$$\psi(O) = \psi(X, Y) \Rightarrow \hat{\beta} = \hat{\beta}^{OLS} = (X^T X)^{-1} X^T Y$$

• A non-parametric, **non-linear** alternative inference is SVM classification. If  $\psi_x \in H$  is the lifting function  $\psi: R^n \rightarrow R^d$  ( $\psi: x \in R^n \rightarrow z = \psi_x \in H$ ) where  $n < d$ , the kernel  $\psi(x, y) = \langle x, y \rangle: O \times O \rightarrow R$  transforms non-linear to linear separation, the observed data  $O_i = \{x_i, y_i\} \in R^n$  are lifted to  $\psi_{x_i} \in H$ . Then, the SVM prediction operator is the weighted sum of the kernel functions at  $\psi_{x_i}$ , where  $\hat{\beta}^*$  is a solution to the SVM regularized optimization:

$$\langle \psi_O | \hat{\beta}^* \rangle_H = \sum_{i=1}^n p_i^* \langle \psi_O | \psi_{x_i} \rangle_H$$

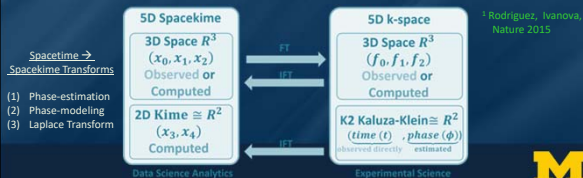
The linear coefficients,  $p_i^*$ , are the dual weights that are multiplied by the label corresponding to each training instance,  $\{y_i\}$ .

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: <http://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<sup>1</sup> 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.



## 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)

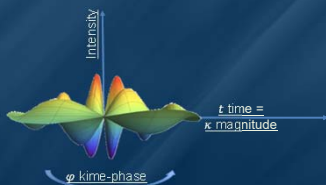
3D pseudo-spacetime reconstruction:

$$f = \hat{h} \left( \begin{matrix} x_1, x_2, \\ \text{space} \end{matrix}, \begin{matrix} t, \\ \text{time} \end{matrix} \right)$$

## 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 ( $\varphi$ ).

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.

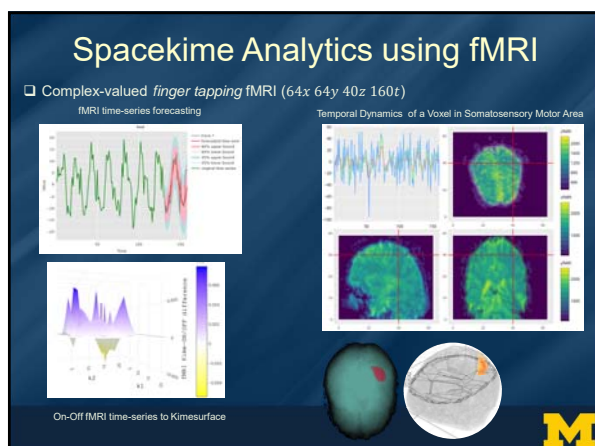


## Bayesian Inference Representation

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

$$\begin{aligned} \frac{p(\gamma|X, \varphi')}{\text{posterior distribution}} &= \frac{p(\gamma, X, \varphi')}{p(X, \varphi')} = \frac{p(X|\gamma, \varphi') \times p(\gamma, \varphi')}{p(X, \varphi')} = \frac{p(X|\gamma, \varphi') \times p(\gamma, \varphi')}{p(X|\varphi') \times p(\varphi')} \\ &= \frac{p(X|\gamma, \varphi')}{p(X|\varphi')} \times \frac{p(\gamma, \varphi')}{p(\varphi')} = \frac{p(X|\gamma, \varphi') \times p(\gamma|\varphi')}{\frac{p(X|\varphi')}{\text{observed evidence}}} \propto \frac{p(X|\gamma, \varphi')}{\text{likelihood}} \times \frac{p(\gamma|\varphi')}{\text{prior}} \end{aligned}$$


- In Bayesian terms, the posterior probability distribution of the unknown parameter  $\gamma$  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,  $x_{i_0}$ .



## 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 data science methods, enhance the computing infrastructure, train/support students/fellows, and tackle the *Kryder Law* >> *Moore Law* trend
- Web: [www.SOCR.umich.edu](http://www.SOCR.umich.edu)
- Git: <https://github.com/SOCR>
- Projects: [www.socr.umich.edu/html/SOCR\\_Research.html](http://www.socr.umich.edu/html/SOCR_Research.html)
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