

Data Sharing + Open, Rigorous & Reproducible Science

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Slides Online: "SOCR News"

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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

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Pillars of Open Data Science (HS650 / Bioinfo501)

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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 (2023) *Springer*

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Native Process (Natural Phenomenon) → **Big Data** (Proxy of the Population) → **Sample Data** (Classical Observations)

Population/Census (Unobservable) → **Big Data** (Harmonize/Aggregate Problems) → **Sample** (Limited process view)

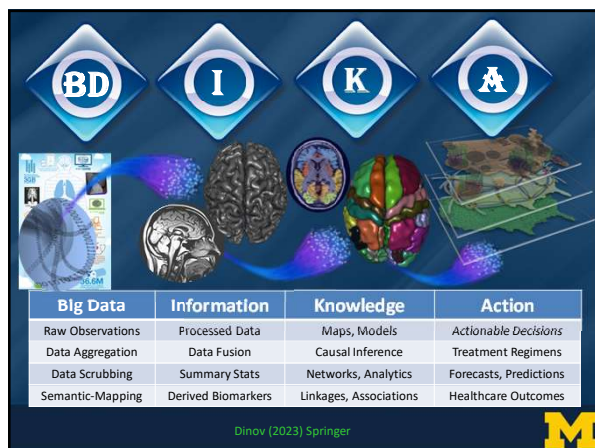
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From 23 ... to ... 2²³

- ❑ Data Science: 1798 vs. 2024
- ❑ 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/H₂O (5.483 ± 0.1904 g/cm³)
- ❑ 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 2²³ bytes
- ❑ Data & Information Science ≅ Scalability & Compression (per Gerald Friedland/Berkeley): 23 → 2²³ ≈ 10M

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

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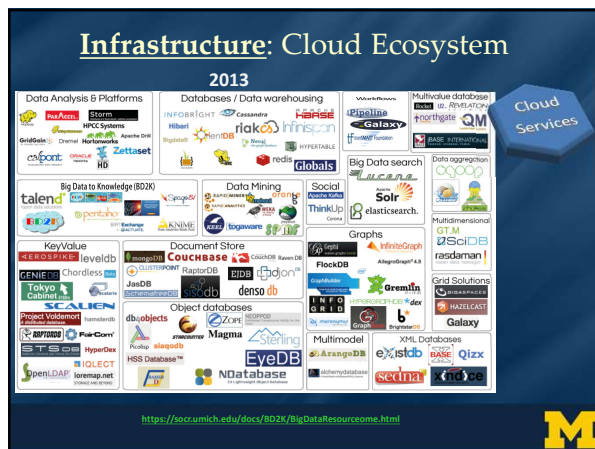
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Why is FAIR Data Sharing Important?

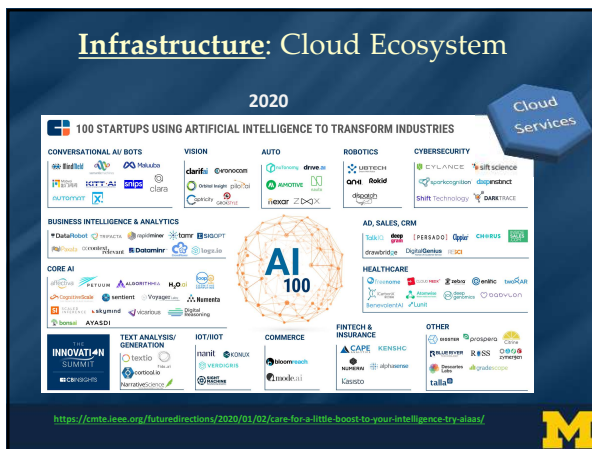
- Optimum resource utilization (low cost, high efficiency / policy, security, processing complexity)
- Democratization of the scientific discovery process
- Enhanced inference (e.g., coverage of rare events, increase of stat power)
- Increase of Kryder's Law (Data volume) \gg Moore's Law (Compute power)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

FAIR = Findable + Accessible + Interoperable + Reusable

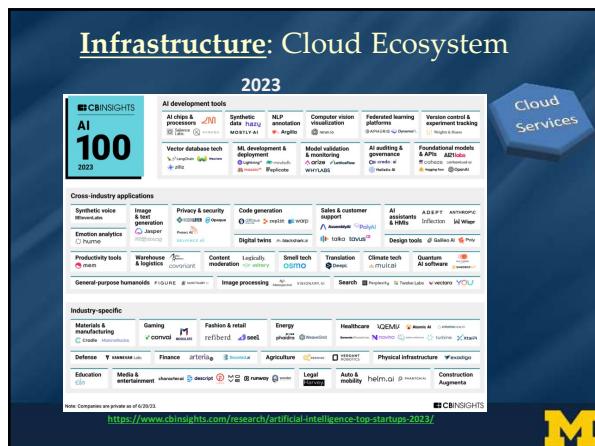
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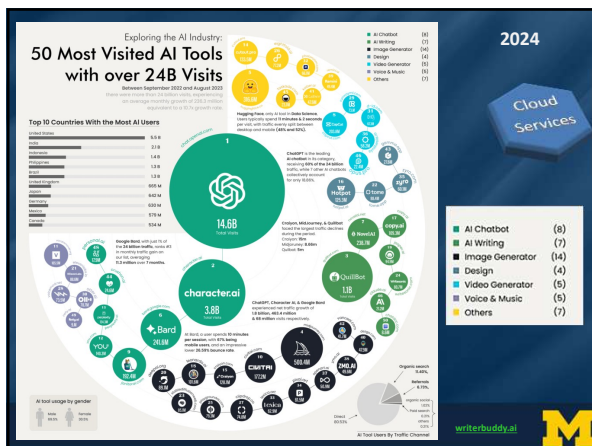
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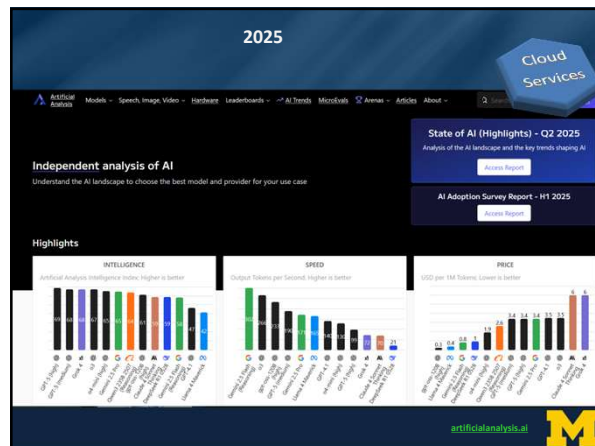
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Scholarly Research: OA Pubs/Sharing

- 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](https://jupyter.org) | [Rmarkdown.rstudio.com](https://rmarkdown.rstudio.com)
 - E.g., <https://DSPA2.predictive.space>
- Licensing
 - <https://www.gnu.org/licenses>
 - https://socr.umich.edu/html/SOCR_CitingLicense.html

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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?

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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, clandestine science, knowledge obfuscation
- ...

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

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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.

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

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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), ...
- Digital Twins: <https://EHR-Sim.StatisticalComputing.org/clinical-phenotype>

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DataSifter

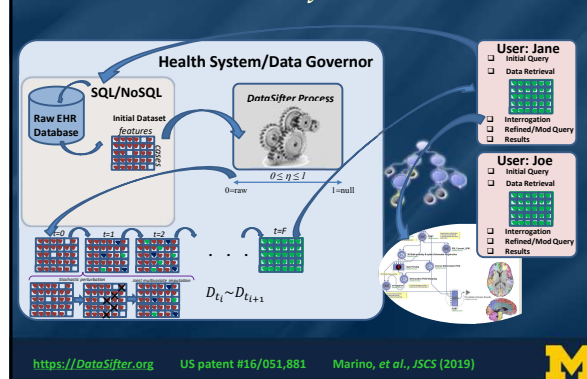
- DataSifter is an iterative statistical computing approach that provides the data-governors controlled manipulation of the trade-off between sensitive information obfuscation and preservation of the joint distribution.
- The DataSifter is designed to satisfy data requests from pilot study investigators 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.

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



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DataSifter



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



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DataSifter Longitudinal Obfuscator

DSLO Data Input

Upload time series data or generate simulated data to analyze

Upload Data Simulate Data

Upload CSV Data

Browse... No file selected.

Required CSV Format:

```

ID,repeatIndex,timeStamp,value,timeStamp_app,diagnosis_type,gender
S10001_0,2023-04-12T15:00:00,08.4002,2,10.000000000000000,1/23/2023,11.00,45,type_3,F
S10001_0,2023-04-12T15:00:00,08.4002,2,1.000000000000000,1/23/2023,11.00,45,type_3,F
S10001_1,2023-04-12T15:00:00,08.4002,4,0.000000000000000,1/23/2023,11.00,45,type_3,F
S10001_1,2023-04-12T15:00:00,08.4002,2,10.000000000000000,1/23/2023,11.00,45,type_3,F
  
```

Column Requirements:

- ID: Identifier for each participant (e.g., S10001)
- repeatIndex: Index for repeated time series (e.g., 0, 1, 2)
- TimeStamp: ISO format timestamp (e.g., 2023-04-12T15:06:10.693Z)
- Value: Numeric value or NaN for missing data points
- TimeStamp: Optional formatted timestamp (e.g., 3/25/2025 11:00)
- Additional Columns: Any static phenotype variables (e.g., age, disease, type, gender) will be included as additional columns. These columns remain constant for each ID.

Try it: <https://SOCR-DSLO.stat.cmu.edu>

<https://www.ukbb.ac.uk>

DataSifter



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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	12138	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	12661	Brain MRI	Reason believed unsafe to perform brain MRI	
100	12704	Brain MRI	Reason brain MRI not completed	
100	12602	Brain MRI	Reason brain MRI not performed	
101	12262	Carotid ultrasound	Carotid ultrasound measurement completed	
101	12291	Carotid ultrasound	Carotid ultrasound measuring method	
101	20235	Carotid ultrasound	Carotid ultrasound results package	
101	22670	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	22678	Carotid ultrasound	Maximum carotid IMT (intima-medial thickness) at 180 degrees	
101	22681	Carotid ultrasound	Maximum carotid IMT (intima-medial thickness) at 210 degrees	
101	22671	Carotid ultrasound	Mean carotid IMT (intima-medial thickness) at 120 degrees	
101	22674	Carotid ultrasound	Mean carotid IMT (intima-medial thickness) at 150 degrees	
101	22677	Carotid ultrasound	Mean carotid IMT (intima-medial thickness) at 180 degrees	
101	22680	Carotid ultrasound	Mean carotid IMT (intima-medial thickness) at 210 degrees	
101	22670	Carotid ultrasound	Minimum carotid IMT (intima-medial thickness) at 120 degrees	
101	22673	Carotid ultrasound	Minimum carotid IMT (intima-medial thickness) at 150 degrees	
101	22676	Carotid ultrasound	Minimum carotid IMT (intima-medial thickness) at 180 degrees	
101	22679	Carotid ultrasound	Minimum carotid IMT (intima-medial thickness) at 210 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

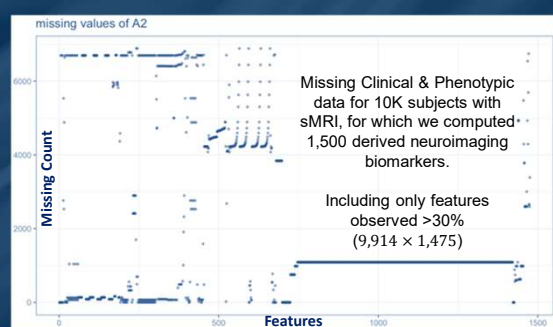
Data Source	Sample Size/Data Type	Summary
UK Biobank	Demographics: > 500K cases Clinical data: > 4K features Imaging data: T1, resting-state fMRI, task fMRI, T2-FLAIR, dMRI, SWI Genetics data	The longitudinal archive of the UK population (NHS)

<https://www.ukbb.ac.uk>
<https://bd2k.org>



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Case-Studies – UK Biobank (Complexities)

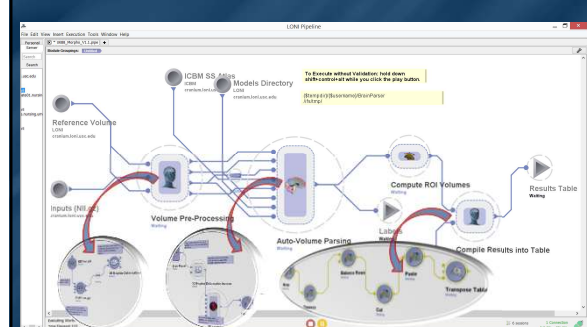


Zhou, et al. (2019), SREP | https://github.com/SOCR/UKBB_Analytics



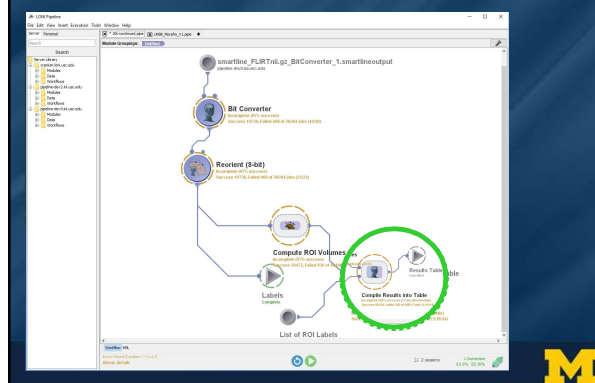
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Case-Studies – UK Biobank – NI Biomarkers



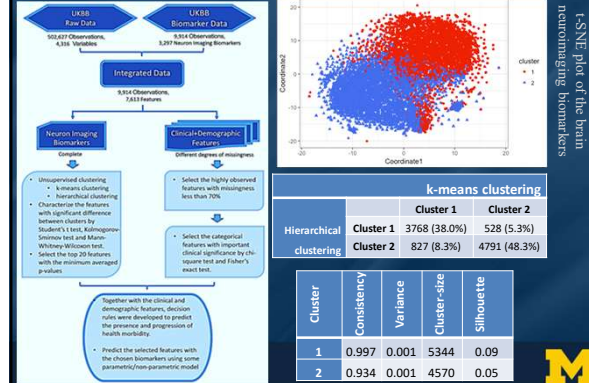
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Case-Studies – UK Biobank – Successes/Failures



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Case-Studies – UK Biobank – Results



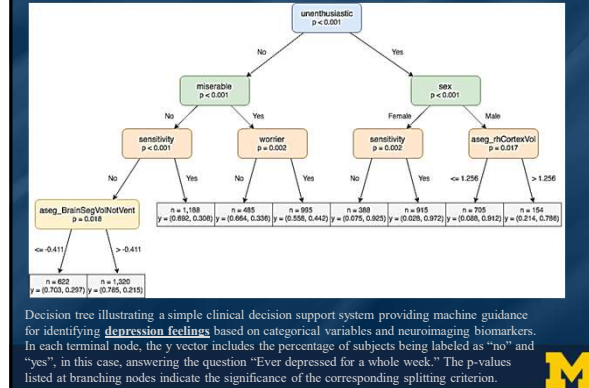
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Case-Studies – UK Biobank – Results

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%)	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%)

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Case-Studies – UK Biobank – Results



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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

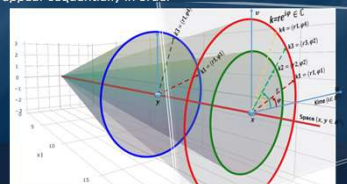
Cross-validated (random forest) prediction results for four types of mental disorders

Zhou, et al. (2019), SREP

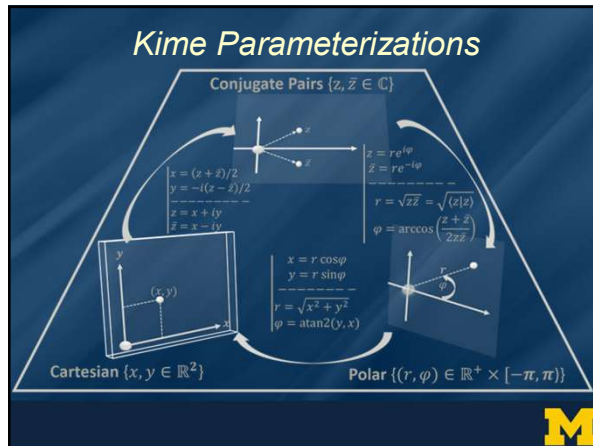
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Complex-Time (Kime)

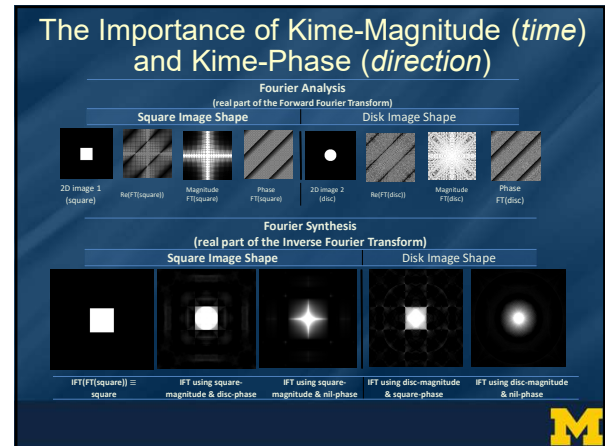
- At a given spatial location, x , complex time (*kime*) is defined by $\kappa = r e^{i\varphi} \in \mathbb{C}$, where:
 - the **magnitude** represents the longitudinal events order ($r > 0$) and characterizes the longitudinal displacement in time, and
 - event **phase** ($-\pi \leq \varphi < \pi$) is an angular displacement, or event direction
- There are multiple alternative parametrizations of kime in the complex plane
- Space-kime manifold is $\mathbb{R}^3 \times \mathbb{C}$:
 - (x, k_1) and (x, k_4) have the same spacetime representation, but different spacetime coordinates,
 - (x, k_1) and (y, k_1) share the same kime, but represent different spatial locations,
 - (x, k_2) and (x, k_3) have the same spatial-locations and kime-directions, but appear sequentially in order



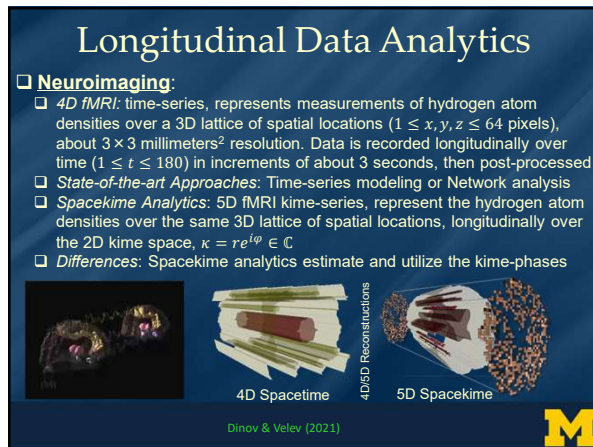
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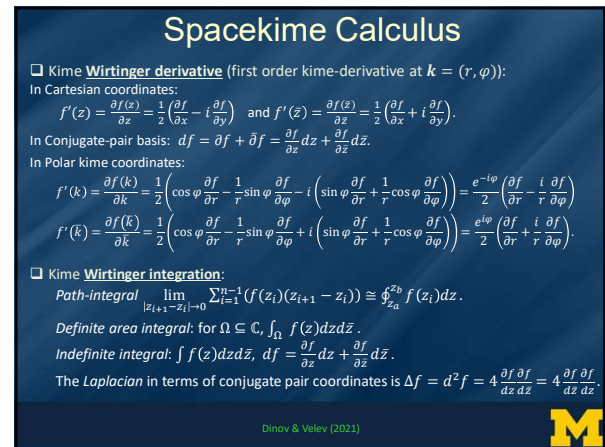
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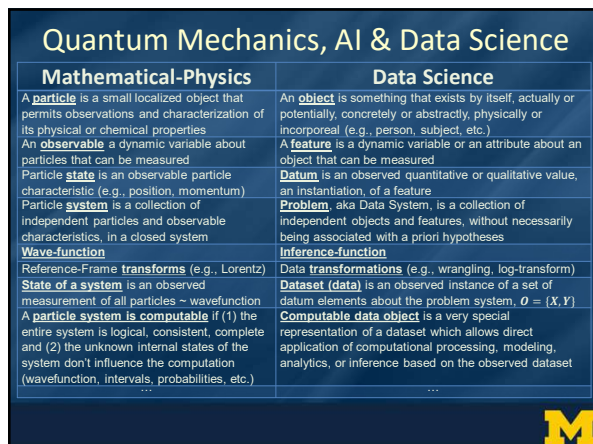
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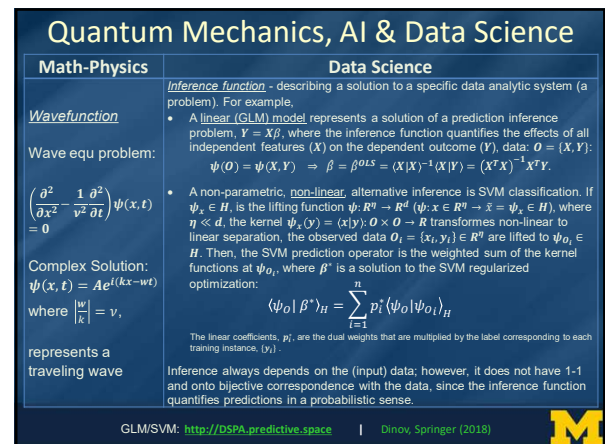
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Spacekime Analytics

- Let's assume that we have:
 - (1) Kime extension of Time, and
 - (2) Parallels between wavefunctions \leftrightarrow 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 crystallographers¹ 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 \rightarrow
Spacekime Transforms

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

5D Spacekime
3D Space R^3
(x_0, x_1, x_2)
Observed or
Computed

2D Kime $\cong R^2$
(x_3, x_4)
Computed

Data Science Analytics

FT

IFT

IFT

Experimental Science

5D k-space
3D Space R^3
(f_0, f_1, f_2)
Observed or
Computed

K2 Kaluza-Klein $\cong R^2$
(time (t), phase (ϕ))
observed directly estimated

¹ Rodriguez, Ivanova, Nature 2015

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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:

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

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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.

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Bayesian Inference Representation

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

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

- 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_{t_0} .

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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

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Try Spacekime Analytics using Sim Data

Time-series to Kime-Surfaces Mapper

Transforming repeatedly sampled time-series data into complex-time (kime) representations for Spacekime Analytics

Web GUI: Interactive Visualizations, Analytic Transforms, Theoretical Background

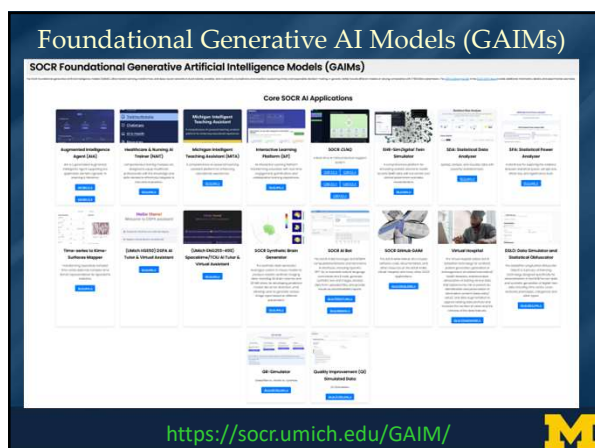
Wave Parameters: Amplitude, Frequency, Phase, Number of Peaks, Time Scale, Base Function, Time, Phase Distribution

Wave Plot

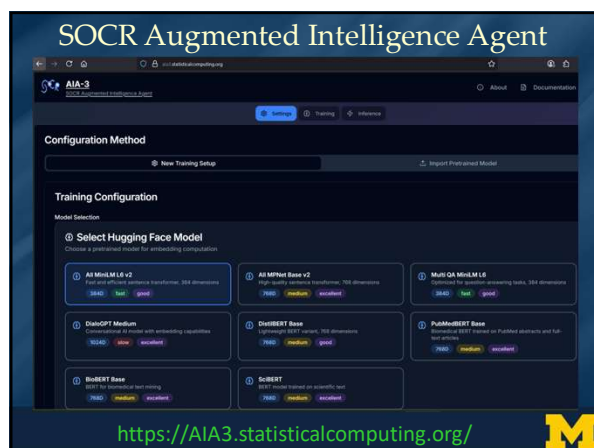
Kime Surface Plot

<https://Kime.StatisticalComputing.org>

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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* >> *Moore Law* trend
- **Web:** www.SOCR.umich.edu
- **Git:** <https://github.com/SOCR>
- **Projects:** www.socr.umich.edu/html/SOCR_Research.html
- **Apps:** <https://socr.umich.edu/HTML5/>

Share

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Acknowledgments

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NSF: 1916425, 1734853, 1636840, 1416953, 0716055, 1023115

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- UMICH MIDAS/MCAIM Centers: Lydia Bieri, Kayvan Najarian, Chris Monk, Issam El Naqa, HV Jagadeish, Brian Athey, Magdalena Ivanova

<https://socr.umich.edu>

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