Computational Neuroscience, Time Complexity & Spacekime Analytics

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Based on an upcoming book "*Data Science: Time Complexity and Inferential Uncertainty*"

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Slides Online:
"SOCR News"

Outline

- Big Neuroscience Analytics Challenges
- Complex-Time (*kime*) & Space-kime Calculus

- Time-series → Kime-Surfaces
- Connection between AI, QM & Data Science

- Statistical Implications of Spacekime Analytics
  Bayesian Inference Representation

- Neuroimaging Applications – Longitudinal Spacekime Data Analytics (UKBB, fMRI)

Common Characteristics of Big Neuro 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 multivariate representation & modeling
Multi-scale	Macro → meso → micro → nano scale observations
Time	Techniques accounting for longitudinal effects (e.g., time corr)
Incomplete	Reliable management of missing data, imputation

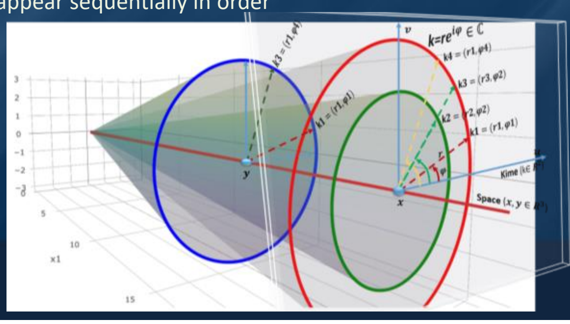
<u>**Example**</u>: analyzing observational data of 1,000's Parkinson's disease patients based on 10,000's signature biomarkers derived from multi-source imaging, genetics, clinical, physiologic, phenomics and demographic data elements

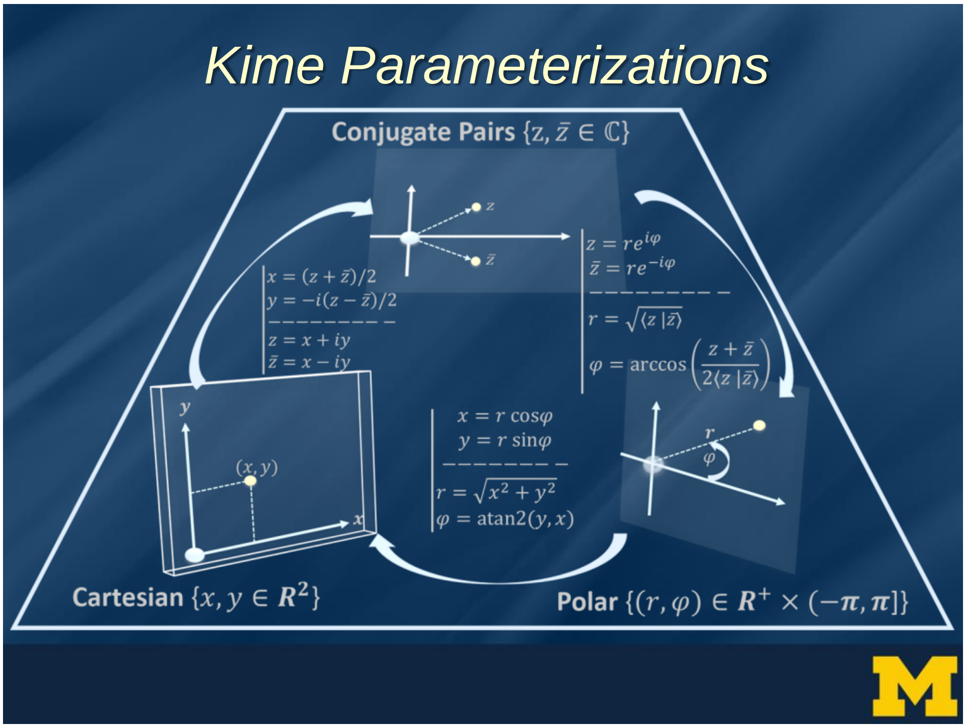
Software developments, student training, service platforms and methodological advances associated with the Big Data Discovery Science all present existing opportunities for learners, educators, researchers, practitioners and policy makers

Dinov, *GigaScience* (2016) PMID:26918190

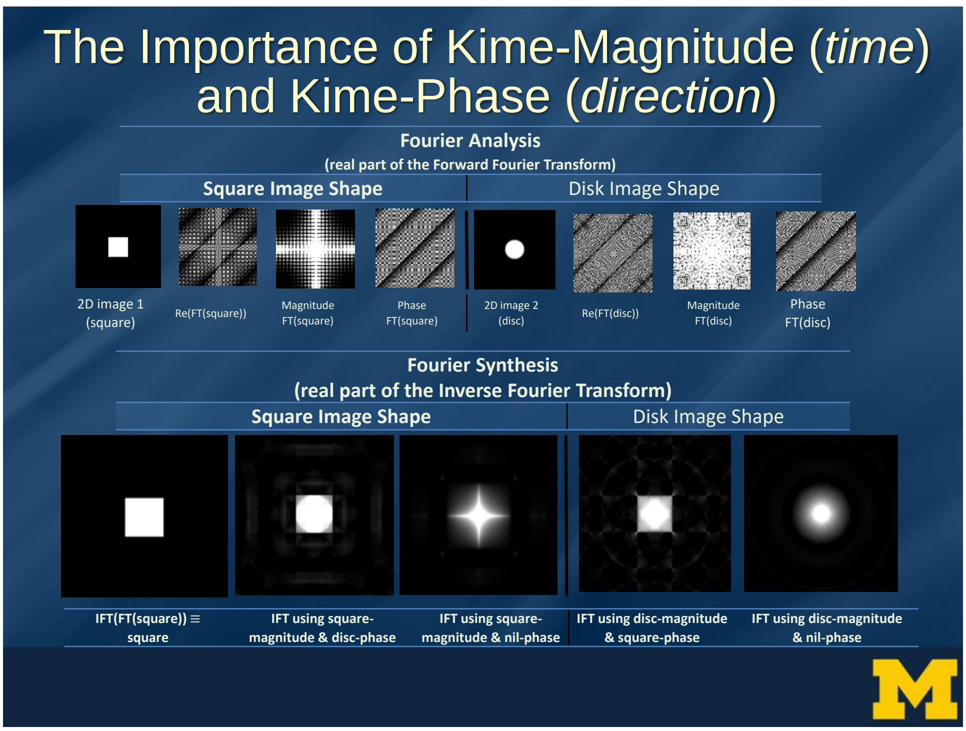
Complex-Time (*Kime*)

- At a given spatial location, $\boldsymbol{x}$, complex time (*kime*) is defined by $\kappa = re^{i\varphi} \in \mathbb{C}$, where:
  - the <u>magnitude</u> represents the longitudinal events order ($r > 0$) and characterizes the longitudinal displacement in time, and
  - event <u>phase</u> ($-\pi \le \varphi < \pi$) 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





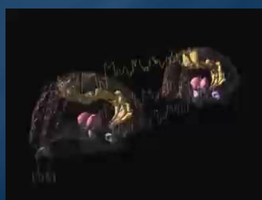
Kime Parameterizations
Conjugate Pairs $\{z, \bar{z} \in \mathbb{C}\}$
$z = re^{i\varphi}$
$\bar{z} = re^{-i\varphi}$
$r = \sqrt{\langle z \mid \bar{z} \rangle}$
$\varphi = \arccos\left(\frac{z+\bar{z}}{2\langle z \mid \bar{z}\rangle}\right)$
$x = (z+\bar{z})/2$
$y = -i(z-\bar{z})/2$
$z = x + iy$
$\bar{z} = x - iy$
$x = r\cos\varphi$
$y = r\sin\varphi$
$r = \sqrt{x^2+y^2}$
$\varphi = \mathrm{atan2}(y, x)$
(x, y)
Cartesian $\{x, y \in R^2\}$
Polar $\{(r, \varphi) \in R^+ \times (-\pi, \pi]\}$

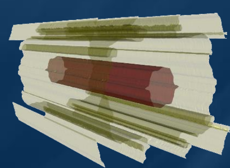


The Importance of Kime-Magnitude (*time*) and Kime-Phase (*direction*)
Fourier Analysis
(real part of the Forward Fourier Transform)
Square Image Shape
Disk Image Shape
2D image 1 (square)
Re(FT(square))
Magnitude FT(square)
Phase FT(square)
2D image 2 (disc)
Re(FT(disc))
Magnitude FT(disc)
Phase FT(disc)
Fourier Synthesis
(real part of the Inverse Fourier Transform)
Square Image Shape
Disk Image Shape
IFT(FT(square)) ≡ square
IFT using square-magnitude & disc-phase
IFT using square-magnitude & nil-phase
IFT using disc-magnitude & square-phase
IFT using disc-magnitude & nil-phase

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 millimeters^2 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





4D Spacetime

4D/5D Reconstructions

5D Spacekime

Dinov & Velev (2021)

Spacekime Calculus

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

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

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

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**:

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

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

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

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, $O = \{X, Y\}$
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: $\left(\frac{\partial^2}{\partial x^2} - \frac{1}{v^2}\frac{\partial^2}{\partial t}\right)\psi(x,t) = 0$ Complex Solution: $\psi(x,t) = Ae^{i(kx-wt)}$ where $\left\vert\frac{w}{k}\right\vert = v$, 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, $Y = X\beta$, where the inference function quantifies the effects of all independent features (X) on the dependent outcome (Y), data: $O = \{X, Y\}$: $\psi(O) = \psi(X,Y) \Rightarrow \hat{\beta} = \hat{\beta}^{OLS} = \langle X \vert X\rangle^{-1}\langle X \vert Y\rangle = (X^T X)^{-1} X^T Y.$ • A non-parametric, non-linear, alternative inference is SVM classification. If $\psi_x \in H$, is the lifting function $\psi: R^\eta \to R^d$ ($\psi: x \in R^\eta \to \tilde{x} = \psi_x \in H$), where $\eta \ll d$, the kernel $\psi_x(y) = \langle x \vert y\rangle: O \times O \to R$ transformes non-linear to linear separation, the observed data $O_i = \{x_i, y_i\} \in R^\eta$ are lifted to $\psi_{O_i} \in H$. Then, the SVM prediction operator is the weighted sum of the kernel functions at ψ_{O_i}, where β^* is a solution to the SVM regularized optimization: $\langle \psi_O \vert \beta^* \rangle_H = \sum_{i=1}^{n} p_i^* \langle \psi_O \vert \psi_{O_i} \rangle_H$ 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 [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

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

FT →
← IFT
← IFT

5D k-space
- 3D Space R^3 (f_0, f_1, f_2) Observed or Computed
- K2 Kaluza-Klein $\cong R^2$ $(\underbrace{time\ (t)}_{observed\ directly}, \underbrace{phase\ (\phi)}_{estimated})$

Data Science Analytics — Experimental Science

[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)

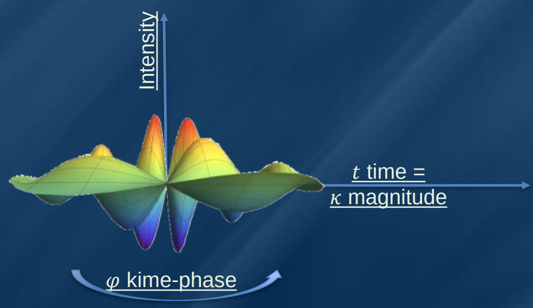
3D pseudo-spacetime reconstruction:

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

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:

$$\underbrace{p(\gamma|X,\varphi')}_{\text{posterior distribution}} = \frac{p(\gamma,X,\varphi')}{p(X,\varphi')} = \frac{p(X|\gamma,\varphi')\times p(\gamma,\varphi')}{p(X,\varphi')} = \frac{p(X|\gamma,\varphi')\times p(\gamma,\varphi')}{p(X|\varphi')\times p(\varphi')} =$$

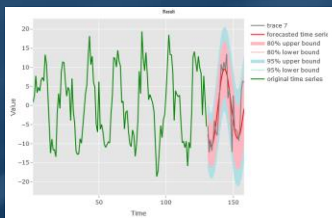
$$= \frac{p(X|\gamma,\varphi')}{p(X|\varphi')}\times\frac{p(\gamma,\varphi')}{p(\varphi')} = \frac{p(X|\gamma,\varphi')\times p(\gamma|\varphi')}{\underbrace{p(X|\varphi')}_{\text{observed evidence}}} \propto \underbrace{p(X|\gamma,\varphi')}_{\text{likelihood}}\times\underbrace{p(\gamma|\varphi')}_{\text{prior}}.$$

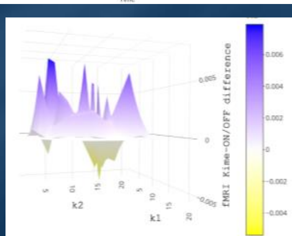
- In Bayesian terms, the posterior probability distribution of the unknown parameter γ is proportional to the product of the likelihood and the prior.
- In probability terms, the posterior = likelihood times prior, divided by the observed evidence, in this case, a single spacetime data point, x_{i_o}.

Spacekime Analytics using fMRI

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

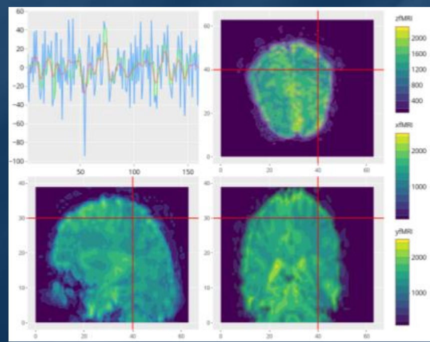
fMRI time-series forecasting

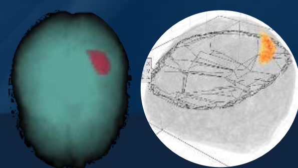




On-Off fMRI time-series to Kimesurface

Temporal Dynamics of a Voxel in Somatosensory Motor Area





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https://Spacekime.org

https://SOCR.umich.edu