Data Science & Predictive Health Analytics

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http://SOCR.umich.edu http://Predictive.Space

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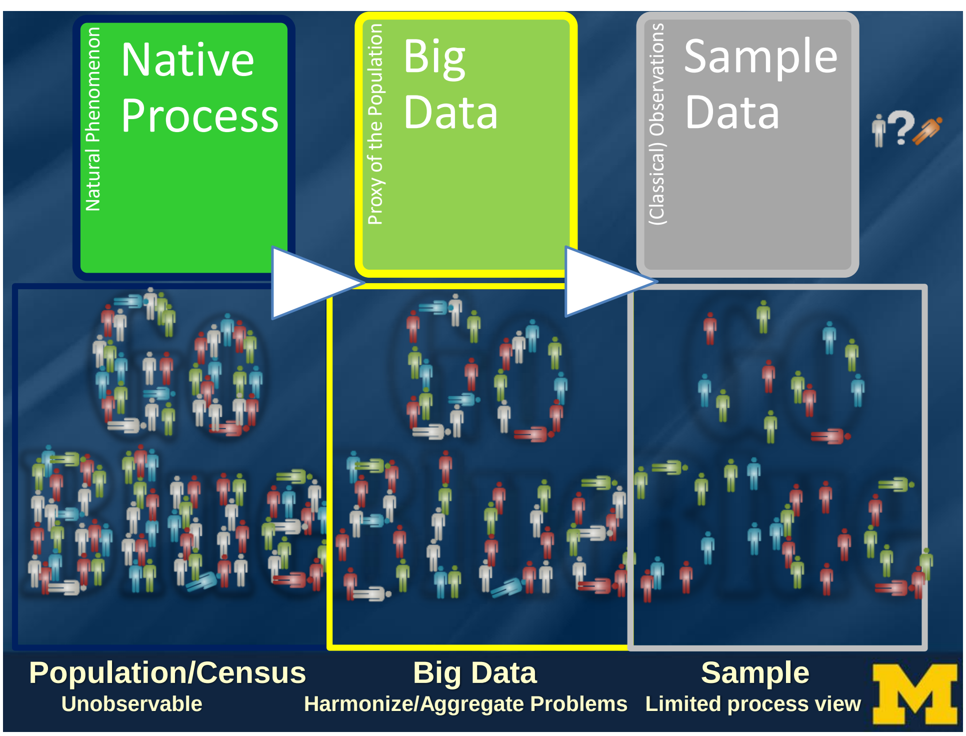
Slides Online:
"SOCR News"

2018 Big Data Summer Institute

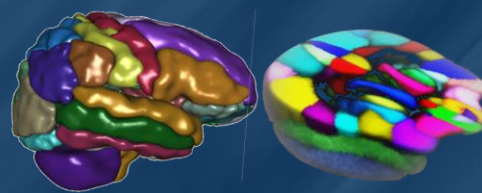
Outline

- Driving biomedical & health challenges
- Common characteristics of Big Biomedical Data
- Data science & predictive analytics
- Compressive Big Data Analytics (CBDA)
- Case-studies
  - Applications to Neurodegenerative Disease
  - Data Dashboarding



Driving Biomedical/Health Challenges

- **Neurodegeneration**: Structural Neuroimaging in Alzheimer's Disease illustrates the Big Data challenges in modeling complex neuroscientific data. 808 ADNI subjects, 3 groups: 200 subjects with Alzheimer's disease (AD), 383 subjects with mild cognitive impairment (MCI), and 225 asymptomatic normal controls (NC). The 80 neuroimaging biomarkers and 80 highly-associated SNPs.



A: Individual brain parcellation — B: LPBA40 atlas

Index	Volume Intensity	ROI Name	Index	Volume Intensity	ROI Name
1	21	L superior frontal gyrus	29	65	L inferior occipital gyrus
2	24	R middle frontal gyrus	30	164	R putamen
3	50	R precuneus	31	61	L superior occipital gyrus
4	181	cerebellum	32	30	R middle orbitofrontal gyrus
5	47	L angular gyrus	33	42	R postcentral gyrus
6	122	R cingulate gyrus	34	27	L precentral gyrus
7	83	L middle temporal gyrus	35	32	R lateral orbitofrontal gyrus
8	90	R lingual gyrus	36	121	L cingulate gyrus
9	81	L superior temporal gyrus	37	31	L lateral orbitofrontal gyrus
10	91	L fusiform gyrus	38	92	R fusiform gyrus
11	44	R superior parietal gyrus	39	45	L supramarginal gyrus
12	66	R inferior occipital gyrus	40	88	R parahippocampal gyrus
13	87	L parahippocampal gyrus	41	22	R superior frontal gyrus
14	162	R caudate	42	29	L middle orbitofrontal gyrus
15	85	L inferior temporal gyrus	43	68	R cuneus
16	182	brainstem	44	62	R superior occipital gyrus
17	43	L superior parietal gyrus	45	33	L gyrus rectus
18	28	R precentral gyrus	46	48	R angular gyrus
19	23	L middle frontal gyrus	47	64	R middle occipital gyrus
20	89	L lingual gyrus	48	84	R middle temporal gyrus
21	41	L postcentral gyrus	49	49	L precuneus

http://DSPA.predictive.space
Moon, Dinov, *et al.* (2015)

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
Incomplete	Reliable management of missing data

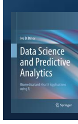
Example: analyzing observational data of 1,000's Parkinson's disease patients based on 10,000's signature biomarkers derived from multi-source imaging, genetics, clinical, physiologic, phenomics and demographic data elements

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, *et al.* (2016) PMID:26918190

Data Science & Predictive Analytics

- **Data Science**: an emerging extremely transdisciplinary field - bridging between the theoretical, computational, experimental, and applied areas. Deals with enormous amounts of complex, incongruent and dynamic data from multiple sources. Aims to develop algorithms, methods, tools, and services capable of ingesting such datasets and supplying semi-automated decision support systems
- **Predictive Analytics**: process utilizing advanced mathematical formulations, powerful statistical computing algorithms, efficient software tools, and distributed web-services to represent, interrogate, and interpret complex data. Aims to forecast trends, cluster patterns in the data, or prognosticate the process behavior either within the range or outside the range of the observed data (e.g., in the future, or at locations where data may not be available)



http://DSPA.predictive.space Dinov, Springer (2018)

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

Case-Studies – ALS

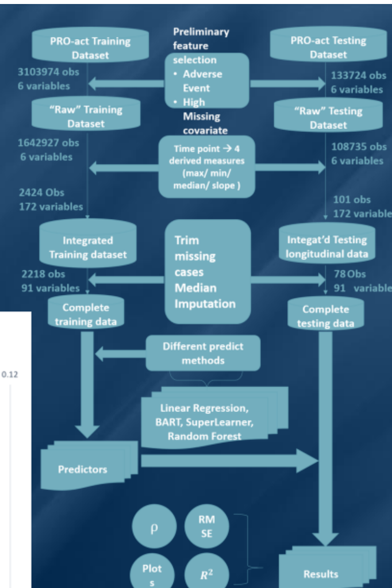
- ❑ Identify predictive classifiers to detect, track and prognosticate the progression of ALS (in terms of clinical outcomes like ALSFRS and muscle function)
- ❑ Provide a decision tree prediction of adverse events based on subject phenotype and 0-3 month clinical assessment changes

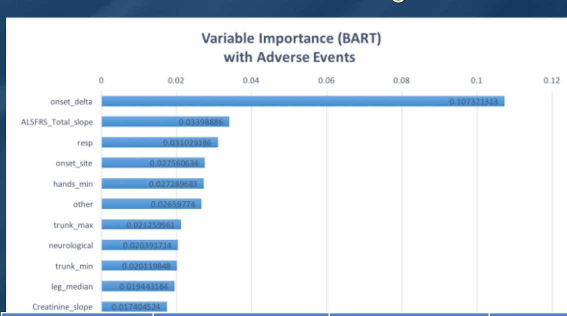
Data Source	Sample Size/Data Type	Summary
ProAct Archive	Over 100 variables are recorded for all subjects including: Demographics: age, race, medical history, sex; Clinical data: **Amyotrophic Lateral Sclerosis** Functional Rating Scale (ALSFRS), adverse events, onset_delta, onset_site, drugs use (riluzole) The PRO-ACT training dataset contains clinical and lab test information of 8,635 patients. Information of 2,424 study subjects with valid gold standard ALSFRS slopes used for processing, modeling and analysis	The time points for all longitudinally varying data elements are aggregated into signature vectors. This facilitates the modeling and prediction of ALSFRS slope changes over the first three months (baseline to month 3)

Tang, et al. (2018), in review

Case-Studies – ALS

- ❑ Detect, track, and prognosticate the progression of ALS
- ❑ Predict adverse events based on subject phenotype and 0-3 month clinical assessment changes





Methods	Linear Regression	Random Forest	BART	SuperLearner
R-squared	0.081	0.174	**0.225**	0.178
RMSE	0.619	0.587	**0.568**	0.585
Correlation	0.298	0.434	**0.485**	0.447

Case-Studies – ALS

- **Main Finding**: predicting univariate clinical outcomes may be challenging, the (information energy) signal is very weak. We can cluster ALS patients and generate evidence-based ALS hypotheses about the complex interactions of *multivariate factors*
- **Classification vs. Clustering**:
  - Classifying univariate clinical outcomes using the PRO-ACT data yields only marginal accuracy (about 70%).
  - Unsupervised clustering into sub-groups generates stable, reliable and consistent computable phenotypes whose explication requires interpretation of multivariate sets of features

Data Representation Fusion Harmonization Aggregation → Cleaning Imputation Wrangling Synthesis → Model-based, Model-free, Classification, Clustering, Inference

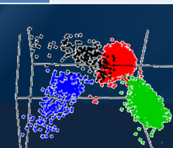
Cluster	Consistency	Variance	Cluster-Size	Silhouette
1	1	0	565	0.58
2	0.986	0.018	427	0.63
3	0.956	0.053	699	0.5
4	0.985	0.018	733	0.5

Tang, et al. (2018), in review

Case-Studies – ALS – Explicating Clustering

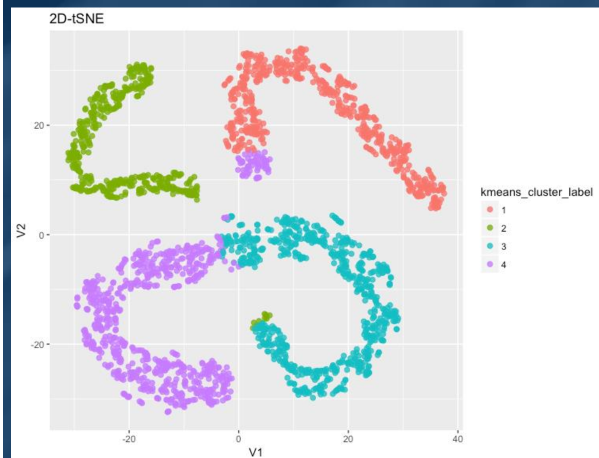
Feature Name	Between Cluster Significant Differences					
	1-2	1-3	1-4	2-3	2-4	3-4
onset_site	[illegible]	[illegible]	1	1	1	
onset_delta.x	1	1	1	1	1	1
onset_delta.y	1	1	1	1	1	
Red.Blood.Cells..RBC._min	1			1	1	
Red.Blood.Cells..RBC._median	1			1	1	
Red.Blood.Cells..RBC._slope				1	1	
Q4_Handwriting_max		1		1	1	
Q4_Handwriting_min		1		1	1	
Q4_Handwriting_median	[illegible]	[illegible]	[illegible]	[illegible]	1	
Q9_Climbing_Stairs_max	[illegible]	1	1	1	1	
Q9_Climbing_Stairs_min		1	1	1	1	
Q9_Climbing_Stairs_median		1	1	1	1	
Q9_Climbing_Stairs_slope	1			1		
Q8_Walking_max		1	1	1	1	
Q8_Walking_min		1	1	1	1	
Q8_Walking_median		1	1	1	1	
trunk_max		1	1	1	1	1
trunk_min		1	1	1	1	
trunk_median		1	1	1	1	
Protein_slope	1			1	1	
Creatinine_max		1	1	1		
Creatinine_min		1	1	1	1	
Creatinine_median		1	1	1	1	
respiratory_rate_max	1			1	1	
hands_max		1		1	1	
hands_min		1		1	1	
hands_median		1		1	1	
Q6_Dressing_and_Hygiene_max		1	1	1	1	
Q6_Dressing_and_Hygiene_min		1		1	1	
Q6_Dressing_and_Hygiene_median		1	1	1	1	
Q7_Turning_in_Bed_max		1	1	1	1	
Q7_Turning_in_Bed_min		1		1	1	
Q7_Turning_in_Bed_median		1	1	1	1	
Sodium_slope	1			1	1	
ALSFRS_Total_max		1		1	1	1
ALSFRS_Total_min		1		1		1
ALSFRS_Total_median		1		1	1	1
ALSFRS_Total_s				1	1	
Hematocrit_max	1			1	1	
Hematocrit_min	1			1	1	
Hematocrit_median	1			1	1	
leg_max		1	1	1	1	
leg_min	[illegible]	[illegible]	1	1	1	
leg_median		1	1	1	1	
mouth_min			1		1	1
Absolute.Basophil.Count_max	1			1	1	
Absolute.Basophil.Count_min	1			1	1	
Absolute.Basophil.Count_median	1			1	1	
Absolute.Basophil.Count_slope	1			1	1	
Absolute.Eosinophil.Count_max	1			1	1	
Absolute.Eosinophil.Count_median	1			1	1	
Absolute.Eosinophil.Count_slope	1			1	1	
Absolute.Lymphocyte.Count_slope	1			1	1	
Absolute.Monocyte.Count_slope	1			1	1	

Feature Name	Between Cluster Significant Differences					
	1-2	1-3	1-4	2-3	2-4	3-4
...	...					
onset_delta.x	1	1	1	1	1	1
...	...					
Q9_Climbing_Stairs_slope	1			1		
...	...					
leg_max		1	1	1	1	
...	...					



Tang, et al. (2018), in review

Case-Studies – ALS – Dimensionality Reduction



2D t-SNE Manifold embedding

Learn a mapping: $f: R^n \xrightarrow{n \gg d} R^d$ $\{x_1, x_2, \ldots, x_n\} \longrightarrow \{y_1, y_2, \ldots, y_d\}$ *preserves* closely the *original distances*, $p_{i,j}$ and represents the *derived similarities*, $q_{i,j}$ between pairs of embedded points:

$$q_{i,j} = \frac{\left(1 + ||y_i - y_j||^2\right)^{-1}}{\sum_{k \neq i}\left(1 + ||y_i - y_k||^2\right)^{-1}}$$

$$\min_f KL(P||Q) = \sum_{i \neq j} p_{i,j} \log \frac{p_{i,j}}{q_{i,j}}$$

$0 = \frac{\partial KL(P||Q)}{\partial y_i} = 2\sum_j (p_{i,j} - q_{i,j}) f(|x_i - x_j|) u_{i,j}$

$f(z) = \frac{z}{1+z^2}$ and $u_{i,j}$ is a unit vector from y_j to y_i.

Tang, et al. (2018), in review

Case-Studies – Parkinson's Disease

- **Investigate falls in PD patients** using clinical, demographic and neuroimaging data from two independent initiatives (UMich & Tel Aviv U)
- Applied **controlled feature selection** to identify the most salient predictors of patient falls (gait speed, Hoehn and Yahr stage, postural instability and gait difficulty-related measurements)
- **Model-based** (e.g., GLM) and **model-free** (RF, SVM, Xgboost) analytical methods used to forecasts clinical outcomes (e.g., falls)
- Internal statistical cross **validation** + external out-of-bag validation
- Four specific **challenges**
  - Challenge 1, harmonize & aggregate complex, multisource, multisite PD data
  - Challenge 2, identify salient predictive features associated with specific clinical traits, e.g., patient falls
  - Challenge 3, forecast patient falls and evaluate the classification performance
  - Challenge 4, predict tremor dominance (TD) vs. posture instability and gait difficulty (PIGD).
- **Results**: model-free machine learning based techniques provide a more reliable clinical outcome forecasting, e.g., falls in Parkinson's patients, with classification accuracy of about 70-80%.

Gao, et al. SREP (2018)

Case-Studies – Parkinson's Disease

Falls in PD are extremely difficult to predict …

PD phenotypes
Tremor-Dominant (TD)
Postural Instability & gait difficulty (PI & GD)

Case-Studies – Parkinson's Disease

Method	acc	sens	spec	ppv	npv	lor	auc
Logistic Regression	0.728	0.537	0.855	0.710	0.736	1.920	0.774
Random Forests	**0.796**	**0.683**	**0.871**	**0.778**	**0.806**	**2.677**	**0.821**
AdaBoost	0.689	0.610	0.742	0.610	0.742	1.502	0.793
XGBoost	0.699	0.707	0.694	0.604	0.782	1.699	0.787
SVM	0.709	0.561	0.806	0.657	0.735	1.672	0.822
Neural Network	0.699	0.610	0.758	0.625	0.746	1.588	
Super Learner	0.738	0.683	0.774	0.667	0.787	1.999	

Results of binary fall/no-fall classification (5-fold CV) using top 10 selected features (gaitSpeed_Off, ABC, BMI, PIGD_score, X2.11, partII_sum, Attention, DGI, FOG_Q, H_and_Y_OFF)

Gao, et al. SREP (2018)

Open-Science & Collaborative Validation

End-to-end Big Data analytic protocol jointly processing complex imaging, genetics, clinical, demo data for assessing PD risk

- Methods for rebalancing of imbalanced cohorts
- ML classification methods generating consistent and powerful phenotypic predictions
- Reproducible protocols for extraction of derived neuroimaging and genomics biomarkers for diagnostic forecasting

https://github.com/SOCR/PBDA

Case-Studies – General Populations

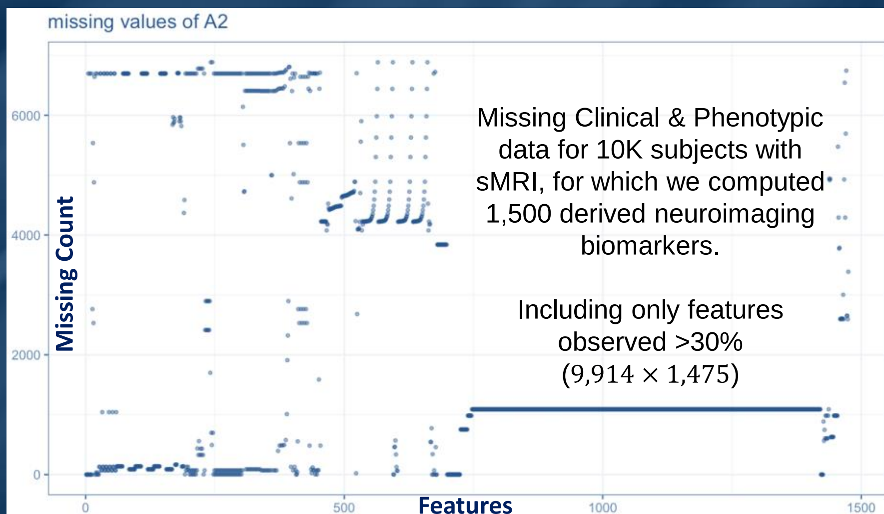
2	20005	Ongoing characteristics	Email access
2	110007	Ongoing characteristics	Newsletter communications, date sent
100	25780	Brain MRI	Acquisition protocol phase.
100	12139	Brain MRI	Believed safe to perform brain MRI scan
100	12188	Brain MRI	Brain MRI measurement completed
100	12187	Brain MRI	Brain 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	22678	Carotid ultrasound	Maximum carotid IMT (intima- degrees
101	22681	Carotid ultrasound	Maximum carotid IMT (intima- degrees
101	22671	Carotid ultrasound	Mean carotid IMT (intima-med
101	22674	Carotid ultrasound	Mean carotid IMT (intima-med
101	22677	Carotid ultrasound	Mean carotid IMT (intima-med
101	22680	Carotid ultrasound	Mean carotid IMT (intima-med
101	22670	Carotid ultrasound	Minimum carotid IMT (intima- degrees
101	22673	Carotid ultrasound	Minimum carotid IMT (intima- 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
101	22684	Carotid ultrasound	Quality control indicator for IMT at 210 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)

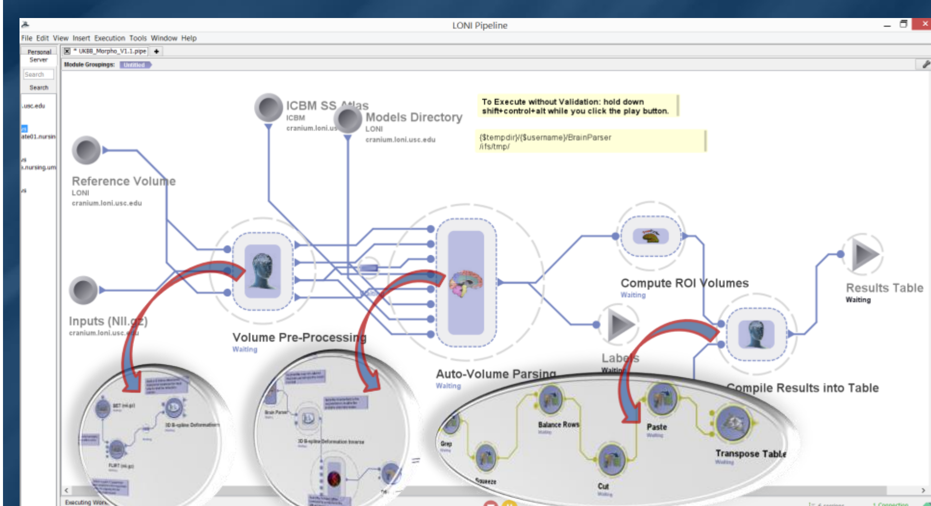
http://www.ukbiobank.ac.uk
http://bd2k.org

Case-Studies – UK Biobank (Complexities)

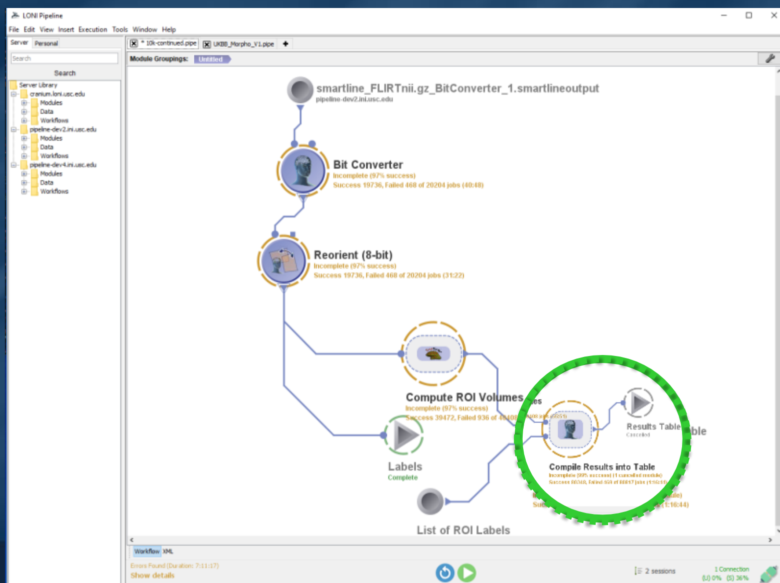


Zhou, et al. (2018), in review

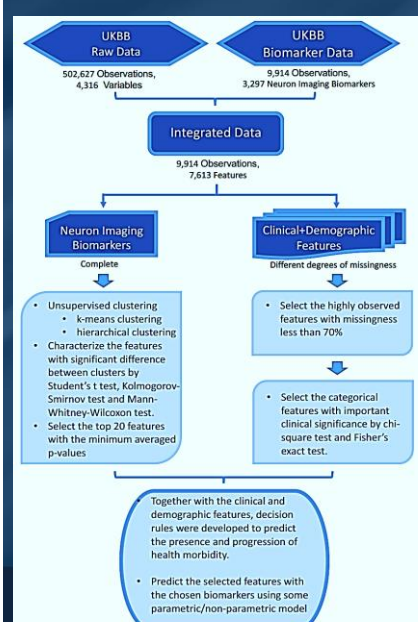
Case-Studies – UK Biobank – NI Biomarkers

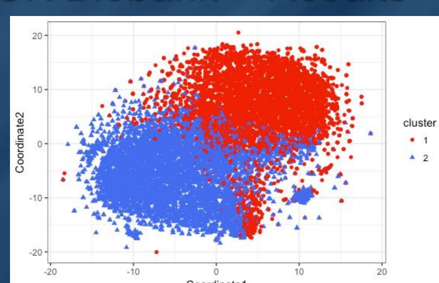


Case-Studies – UK Biobank – Successes/Failures



Case-Studies – UK Biobank – Results





t-SNE plot of the brain neuroimaging biomarkers

		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.[illegible])
Male	3,461 (75.3%)	1,257 (23.[illegible])
Sensitivity/hurt feelings		
Yes	2,142 (47.9%)	3,023 (58.[illegible])
No	2,332 (52.1%)	2,151 (41.[illegible])
Worrier/anxious feelings		
Yes	2,173 (48.2%)	2,995 (57.[illegible])
No	2,337 (51.8%)	2,208 (42.[illegible])
Risk taking		
Yes	1,378 (31.0%)	1,154 (22.[illegible])
No	3,064 (69.0%)	3,933 (77.[illegible])
Guilty feelings		
Yes	1,100 (24.4%)	1,697 (32.[illegible])
No	3,417 (75.6%)	3,536 (67.[illegible])
Seen doctor for nerves, anxiety, tension or depression		
Yes	1,341 (29.3%)	1,985 (37.[illegible])
No	3,237 (70.7%)	3,310 (62.[illegible])
Alcohol usually taken with meals		
Yes	1,854 (66.7%)	2,519 (76.[illegible])
No	924 (33.3%)	771 (23.4[illegible])
Snoring		
Yes	1,796 (41.1%)	1,652 (33.[illegible])
No	2,577 (58.9%)	3,306 (66.[illegible])
Worry too long after embarrassment		
Yes	1,978 (44.3%)	2,675 (52.[illegible])
No	2,491 (55.7%)	2,462 (47.[illegible])
Miserableness		
Yes	1,715 (37.7%)	2,365 (45.[illegible])
No	2,829 (62.3%)	2,882 (54.[illegible])
Ever highly irritable/argumentative for 2 days		
Yes	485 (10.7%)	749 (14.5%)
No	4,038 (89.3%)	4,418 (85.[illegible])
Nervous feelings		
Yes	751 (16.6%)	1,071 (20.[illegible])
No	3,763 (83.4%)	4,076 (79.[illegible])
Ever depressed for a whole week		
Yes	2,176 (48.1%)	2,739 (52.[illegible])
No	2,347 (51.9%)	2,438 (47.[illegible])
Ever unenthusiastic/disinterested for a whole week		
Yes	1,346 (30.3%)	1,743 (34.[illegible])
No	3,089 (69.7%)	3,344 (65.[illegible])
Sleepless/insomnia		
Never/rarely	1,367 (29.8%)	1,181 (22.[illegible])
Sometimes	2,202 (47.9%)	2,571 (48.[illegible])
Usually	1,024 (22.3%)	1,563 (29.[illegible])
Getting up in morning		
Not at all easy	139 (3.1%)	249 (4.7%[illegible]
Not very easy	538 (11.9%)	830 (15.8[illegible]
Fairly easy	2,327 (51.4%)	2,663 (50.[illegible])
Very easy	1,526 (33.7%)	1,505 (28.[illegible])
Nap during day		
Never/rarely	2,497 (54.5%)	3,238 (61.[illegible])
Sometimes	1,774 (38.8%)	1,798 (34.[illegible])
Usually	307 (6.7%)	228 (4.3%[illegible]
Frequency of tiredness/lethargy in last 2 weeks		
Not at all	2,402 (53.0%)	2,489 (47.[illegible])
Several days	1,770 (39.0%)	2,127 (40.[illegible])
More than half the days	187 (4.1%1)	300 (5.8%[illegible]
Nearly everyday	177 (3.9%)	287 (5.5%[illegible]
Alcohol drinker status		
Never	81 (1.8%)	179 (3.4%[illegible]
Previous	83 (1.8%)	146 (2.7%[illegible]
Current	4,429 (96.4%)	[illegible].9%)

Variable	Cluster 1	Cluster 2
Sex		
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…	…	
Nervous feelings		
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No	3,763 (83.4%)	4,076 (79.2%)
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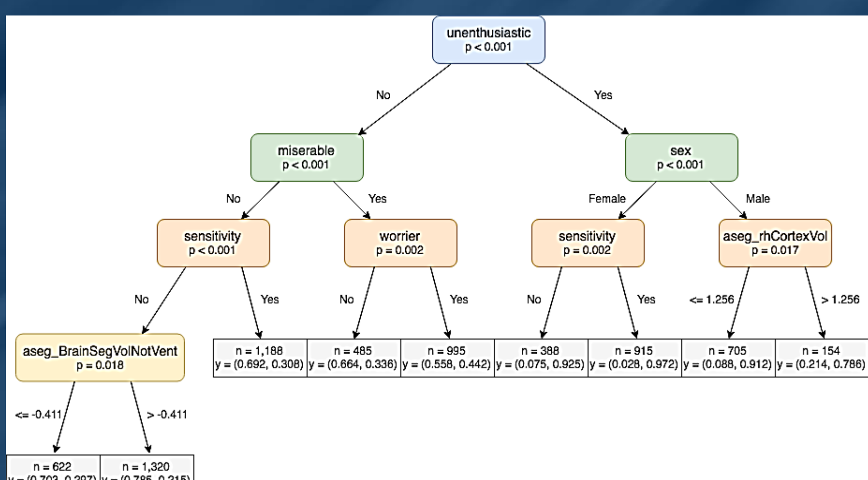
Nearly everyday	177 (3.9%)	287 (5.5%)
Alcohol drinker status		
Never	81 (1.8%)	179 (3.4%)
Previous	83 (1.8%)	146 (2.7%)
Current	4,429 (96.4%)	4,992 (93.9%)

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. (2018), in review

Compressive Big Data Analytics (CBDA)

- Foundation for Compressive Big Data Analytics (CBDA)
  - Iteratively generate random (sub)samples from the Big Data collection
  - Then, using classical techniques to obtain model-based, model-free, non-parametric inference based on the sample
  - Next, compute likelihood estimates (e.g., probability values quantifying effect sizes, relations, and other associations)
  - Repeat – the process continues iteratively until a convergence criterion is met – the (re)sampling and inference steps many times (with or without using the results of previous iterations as priors for subsequent steps)

Dinov, *2016, PMID: 26998309;* *Marino, et al., 2018 (in review)*

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