Current Status and Future Trends in Data Centric Science

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Science Today Is Data Centric





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Hypotheses are discovered in Data and drive Theory



Computation







Experiment

Computations inform the design of Experiments

Datafication Turns Sciences into Data Science



Digitalisation vs Datafication

Digitalisation: is a process that has been active within society since the late 1950s, with the birth of the emiconductor industry. It refers to the conversion of pieces of information into digital formats, for example text into HTML pages, music into MP3s, images into JPEG or similar. As the process of digitalisation has progressed, the amount of data that could be processed has increased exponentially. Digitalisation, therefore, from a simplistic perspective may be viewed as the embodiment of idea creation – it is capturing human ideas in digital form for transmission, re-use and manipulation

Datafication relates to the use of digital technologies to unembed the knowledge associated with physical objects by decoupling them from the data associated with them. Datafication is manifesting itself in society in a variety of forms and is often – but not always – associated with sensors/actuators and the emerging Internet of Things (IoT). Datafication may take many forms and in many cases a mobile device is enough to create unembedded knowledge of a person, a thing or a piece of infrastructure.

Ericssion White Paper : Impact of Datafication on the Strategic Level

Example: Dataficating Life



Google Glass is a camera, display, touchpad, battery and microphone built into spectacle frames so that you can perch a display in your field of vision, film, take pictures, search and translate on the go.



APPLE SMARTWATCH

A wrist-based gadget that can sync with your phone, display information, play music and function similarly to a smartphone.

Wearable camera takes automatic photos of life as it happens which can be searched and shared through Memoto's mobile and web application.





Technology

- _ Wearable sensors: capturing personal physiological and behavioural information
- Cloud: data analysis

Impact

- Enabling **real-time** health monitoring and
- behaviour characterisation
- _ The foundation: personalisation of products and services

Future trends

- Ecosystem: personalised services
- _ Integrated data products: combined with
- personal biological data for **personalised** medicine
- Real-time decision support: **mobile health** monitoring

Technologies for Data Centric Science



41 of Data Centric Science

- Integration: Integrating data for system analysis
- Intelligence: Machining learning for deep understanding and prediction
- Interaction: Integrating data with models and physical systems for adaptive analysis
- Inter-discipline: Understanding complexity by crossdisciplinary study with data as glue

Being Data Centric => Integrative Analysis

- Data centric research requires to collecting data measuring the various aspects of a physical system
- Collected measurements are required to be calibrated and meaningfully integrated.
- The meaningful integration explores the inherent relationships of different modalities of data
- Exploration the relationship requires deep analysis and curation
- Data integration is the core of "Web Science"

BIOLOGY AS DATA SCIENCE

- Genomics
- Proteomics
- Metabolomics
- Phenome





The ABI QSTAR® Pulsar Hybrid LC/MS/MS System is a high performance hybrid quadrupole time-of-flight mass spectrometer







Biology is now a data science



Medicine is now a data science

Google Maps: GIS layers Organized by Geographical Positioning Information Commons Organized Around Individual Patients



Translational Research : Computing Correlations Human Data Size ~ 3.3 billion BPs [29] DNA Variants >62 million SNPs [30] miRNA Expression $> 10^8 \, Cp_$ sites [15] >18 000 non-coding RNAs [28] 10⁸ histone tails [15] DNA Epigenetic Variants mRNA Expression n individual Protein Expression >20 000 protein coding genes [28] samples Metabolic Profile >2500 metabolites [32] Phenotype Environment Any observable traits Diet [32]: > 1200 drugs > 3500 food components + many other factors (e.g. geolocation[33], early-life socioeconomic position[34]) **Combinatorial Explosion** р a **Response matrix:** Predictor matrix: n n

n observations

q variables

Aim: identify which of the p variables in X are significantly associated with the outcome Y

n observations

p variables

Data Driven Medicine: Searching associations



Being Data Centric => Intelligent Analysis

- Data Centric means discovery and predictive
- Discovery requires machine to discover patterns and trends beyond statistical analysis
- Predictive requires machine to build models exploiting the insight from data
- The era of "Machine Science" is coming

(king et al, "The Automation of Science", Science 3 April 2009, Schmidt M and Lipson H, "Distilling Free-Form Natural Laws from Experimental Data", Science 3 April 2009) Alternator

Big Algorithm + Small Data: Exploring the Local Causality

GasInTank

GasGauge

Sophisticated algorithms and small data:

- Representative sampling (N=k)
- High quality data
- Sophisticated multivariate learning algorithms
- Exploring causality relationships



Small Algorithm + Big Data: Exploring Global Correlation

Simple algorithms and big data:

- Taking all the data (N=all)
- Messy data tolerance
- Simple/scalable learning algorithms
- Exploring correlation relationships



fMRI : Datafication of Brain Function

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HENRY M. WORKSON, S.

DIAMAGNETIC CKTHEWORK

~150,000 locations (voxels) in 2s/time
>100 times
Many experimental conditions
Many participants
Millions of reads and billions of pairwise relations



OKYGEN

Interested of Concession, Manual HENRY H. WHEELER, JR. BRAIN IMAGING CENTER

DOMEMORY DRAW

13

Land I

12

fMRI Analysis



Small Data

Big Data

Big Algorithms + Big Data : Cognition



Deep Learning: From Vision to Cognition



Machine Intelligence Drives the Analytical Technology towards Cognition



Technology

_ Deep learning, Secure learning and NLU

Impact

_ Unlimited, centralised analytics/computing capacity

- Knowledge discovery in real time with big data

Future trends

- _ Machine cognition
- _ Machine Science
- -- Real time discovery
- -- Model based knowledge economy

Being Data Centric => Let Data Speak

- Data Centric requires data to be interactive with other entities in the research (models, physical world and human)
- Such interaction enables adaptive decision making
- The adaptions include : sampling strategies, model parameters, visual understanding
- Interaction suggests a "Data Chemistry"!

WIKIHEALTH : AN INTEGRATED PLATFORM FOR WEARABLE SENSOR INFORMATICS

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The Activities	Days Week Month Year	Upload Status	Clemon Crimina Inscot St. R. R.	Next S Heart-rate
현 EEG	Activity Summary 8744.00 steps taken	Local Database Capacity: 0.2	Du Cane Rd st	Upload
steps	3.00 floors climbed	Upload	Pioneer Way	
🔯 Distance Traveled	1793.91 calories burned	Latest Uploads	A40 Westway	Latest Uploads
Calories Burned	95.14 times per minute Steps:	05/09/2013 - 05:32 05/09/2013 - 01:38	Wood	30/08/2013 - 07:39
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Body Fat Percentage		😵 Sensors 📃	😵 Add Events 📃	🛞 Add Events
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Weight (0kg) 51 137+	Daniel went Time to fall Times awakened Daniel in bed for \$8:57 PM Step awakened Actual 8:57 PM 10mins 20 8hrs 23mins 5:20 AM 7hrs 12mins 2013-02-18	Z-axis 6.65	3:32-4:32 : Writing final project report.	love not coming men project reports

Wiki-Health: Assimilation with human physiology models

- Example of simulating full body temperatures and energy transformation
- Core body temperature & Safety
 - Too high: heat exhaustion, heatstroke
 - Too low: hypothermia





- Age: 27, Weight: 80kg
- 1- 60 min running at a speed of 6mph with air temperature 30°C
- > 60-120 min sit still with air temperature 42°C
- 120-180 min sit still with air temperature 10°C
- 180-240 min running at a speed of 6mph with air temperature 10°C

Chemistry and Data Chemistry

n. The study of the composition, structure, properties, and reactions of matter data (everything that makes up the universe knowledge).

The Basic Concept of Data Chemistry

- Element types : data, model
- Properties:
 - Semantics
 - Provenance
- Structures:
 - Representation
 - Relation
 - Distributionn (Statistics)
- Reaction:
 - Data-data reaction : integration
 - Data-model reaction : assimilation
 - Model-model reaction : knowledge network
- Derivatives :
 - Data exhausts
 - Models

Data/Model Interaction Is Essential in Data Product Innovation



Being Data Centric => Data as Glue

- Datafication made the interaction and integration of scientific disciplines easier
- Data enables a systematic research of a complex system through integrative analysis
- System to system level integration can be achieved via data/model interaction
- Inter-disciplinary research is changing the research organisation structure.

Digital City Exchange : Exploring Data Economy of Smart City



City Air Quality Research Traffic flow, car emission data and weather condition will generate a dynamic map for the air quality of a city.



Building Data Products with Urban Informatics structure





Concinnity: The Digital City Exchange platform

- A generic sensor data management platform "Concinnity" [1] built on Wikisensing [2] datastore and Wikimodelling [3] model integration workflow engine
- 3 layers targeting different stages of the data lifecycle
- Data products built using the application development environment

Concinnity



[1] Lee, C-H, David Birch, Chao Wu, Dilshan Silva, Orestis Tsinalis, Yang Li, Shulin Yan, Moustafa Ghanem, and Yike Guo. "Building a Generic Platform for Big Sensor Data Applications." *Proceedings of the IEEE Big Data conference* (2013), Santa Clara, CA, USA.

[2] Silva, Dilshan, Moustafa Ghanem, and Yike Guo. "WikiSensing: An Online Collaborative Approach for Sensor Data Management." Sensors, 12, no. 10 (2012): 13295-13332.

[3] Birch, David, Paul HJ Kelly, Anthony J. Field, and Alvise Simondetti. "Computationally unifying urban masterplanning." *Proceedings of the ACM International Conference on Computing Frontiers*, p. 32. 2013.

Semantics Engine : Model and Data integration

- Allows workflows to reflect the hierarchies
 - Geographically in the city
 - Temporally in data streams
- Multi-scale analysis and data integration is enabled





Imperial College Data Science Institute: A Focal Point



Conclusion

- Datafication drives the era of data centric science
- Data centric science has the 4I characters : Integrative, interactive, intelligent and interdisciplinary
- Efforts are being made on the development of the 41 technology
- 4I of data centric science are not only technical issues but impact to the research organisation structure
- Data Science Institute of IC aims to develop 4I to explore Big Data for Better Science