







Data in Science versus Data Science: What's the difference?

Chris Stephens

C3-Centro de Ciencias de la Complejidad Instituto de Ciencias Nucleares, UNAM

Data Mining Course, Universidad de Pamplona 4-6 December 2017



- 1. Why do we need data in science?
- 2. Isn't all science "data science"?
- 3. Why do we talk about data science now?
- 4. What's the difference?



The principal purpose of living systems and the principal purpose of science is to...

Predict

for

Decision making



From the science of yesterday to the science of tomorrow...



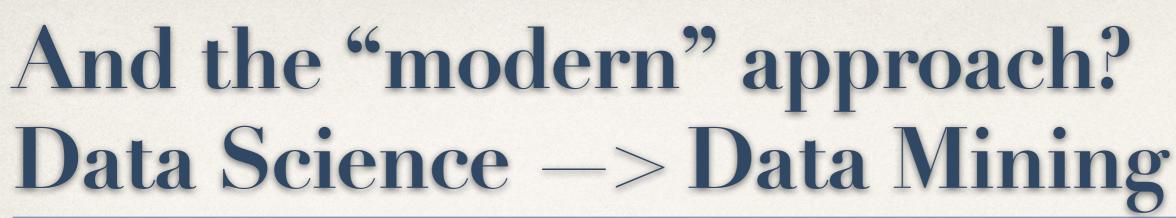
How we do science in a nutshell... The traditional approach

- The Scientific method:

 DATA and DATA of hypotheses

 DATA

 DATA
 - * **Phenomenology** a body of knowledge that relates <u>empirical observations</u> of <u>phenomena</u> to each other, in a way that is *consistent* with fundamental <u>theory</u>, but is not directly derived from theory.
 - * **Taxonomy** the practice and science of classification. A classification of things or concepts, as well as to the principles underlying such a classification.
- DATA * Examples: Medicine, astronomy, chemistry, biology, physics,...
 - * Scientific law when a particular phenomenon always occurs if certain conditions are present





"... the exploration and analysis of data in order to discover patterns, correlations and other regularities."

There are two main datamining tasks

Predicting – "pattern" identification Establishes "causal" statistical relations

Profiling - "pattern" description

Identifies what are the key drivers associated with a pattern

There are three main requirements

Data; "data processors"; "inference algorithms"

The worldview of the last 3 (2)3 centuries:



NO EKCEPTIONS.



we are slaves of the law

Universality We're all equal under the law

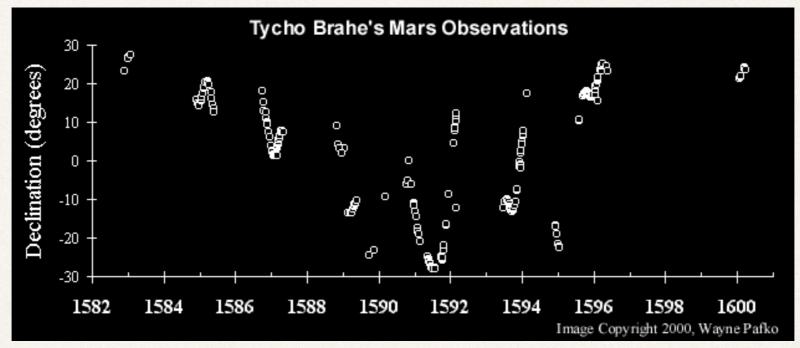


onthere's really not them the tages as At ayounvessend them places that much data

Isn't all Science Data Science?



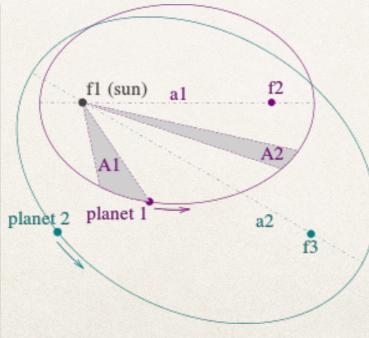














Phenomenology

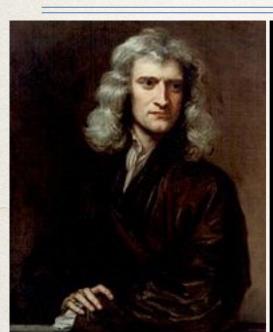
Kepler's Laws

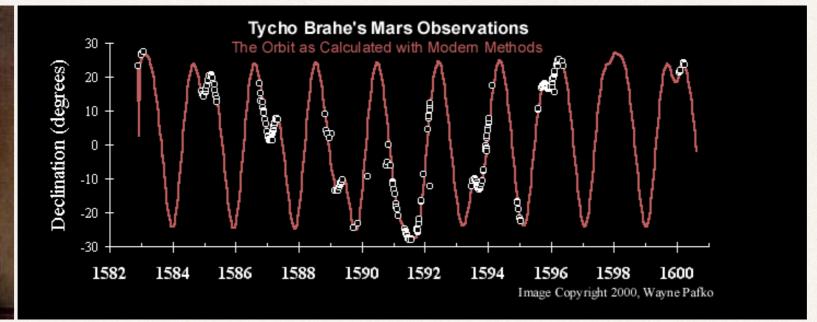
- 1. The orbit of a planet is an ellipse with the Sun at one of the two foci.
- 2. A line segment joining a planet and the Sun sweeps out equal areas during equal intervals of time.
- 3. The square of the orbital period of a planet is proportional to the cube of the semi-major axis of its orbit.

Isn't all Science Data Science?



Data —> Phenomenology —> Taxonomy —> Theory





Theory

F = ma $F = GMm/r^2$

Isaac Newton computed the acceleration of a planet moving according to Kepler's first and second law.

- 1 The direction of the acceleration is towards the Sun.
- 2 The *magnitude* of the acceleration is inversely proportional to the square of the planet's distance from the Sun (the *inverse square law*).

This implies that the Sun may be the physical cause of the acceleration of planets.

Newton defined the force acting on a planet to be the product of its mass and the acceleration. So:

- 1 Every planet is attracted towards the Sun.
- 2 The force acting on a planet is in direct proportion to the mass of the planet and in inverse proportion to the square of its distance from the Sun.

The Sun plays an unsymmetrical part, which is unjustified. So he assumed, in Newton's law of universal gravitation:

- 1 All bodies in the solar system attract one another.
- 2 The force between two bodies is in direct proportion to the product of their masses and in inverse proportion to the square of the distance between them.

As the planets have small masses compared to the Sun, the orbits conform approximately to Kepler's laws. Newton's model fits actual observations more accurately.



Science Data Science?

- * **Data**: Brahe provided an accurate (for the time) data base with data on the positions of different celestial bodies as a function of time.
- Phenomenology: Kepler was a data miner, a data scientist. He mined Brahe's data and inferred regularities and constructed phenomenological models (his three laws) that embodied these regularities.
- **Theory**: Newton used Kepler's laws to construct a theoretical, "universal" model for the gravitational interaction. He <u>inferred</u> the existence and nature of an interaction between objects.
- Where things are as a function of space and/or time allows us to infer the nature of their interactions.
 - By observing the spatio-temporal behaviour of different types of inanimate "things" we have deduced that in the physical world there are 4 interaction types and they are important at quite different scales.
 - There are only very few properties/labels of "things" that are associated with the different interactions: mass, electric charge, weak isospin, colour
 - These interactions DO NOT change!



Data then versus data now

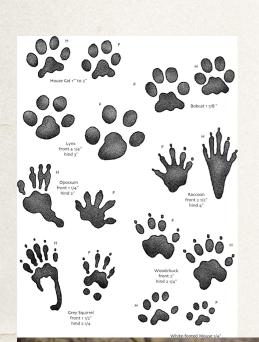
There's been a data revolution...

But just what's revolutionary?



Data types? No.





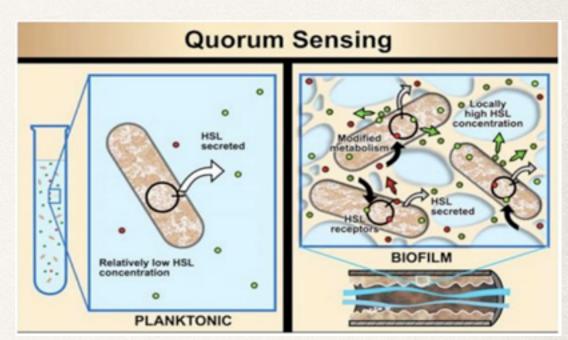
Raw data:

Chemical

Electromagnetic

Acoustic...

as functions of space and time tell us what is going on in the world.



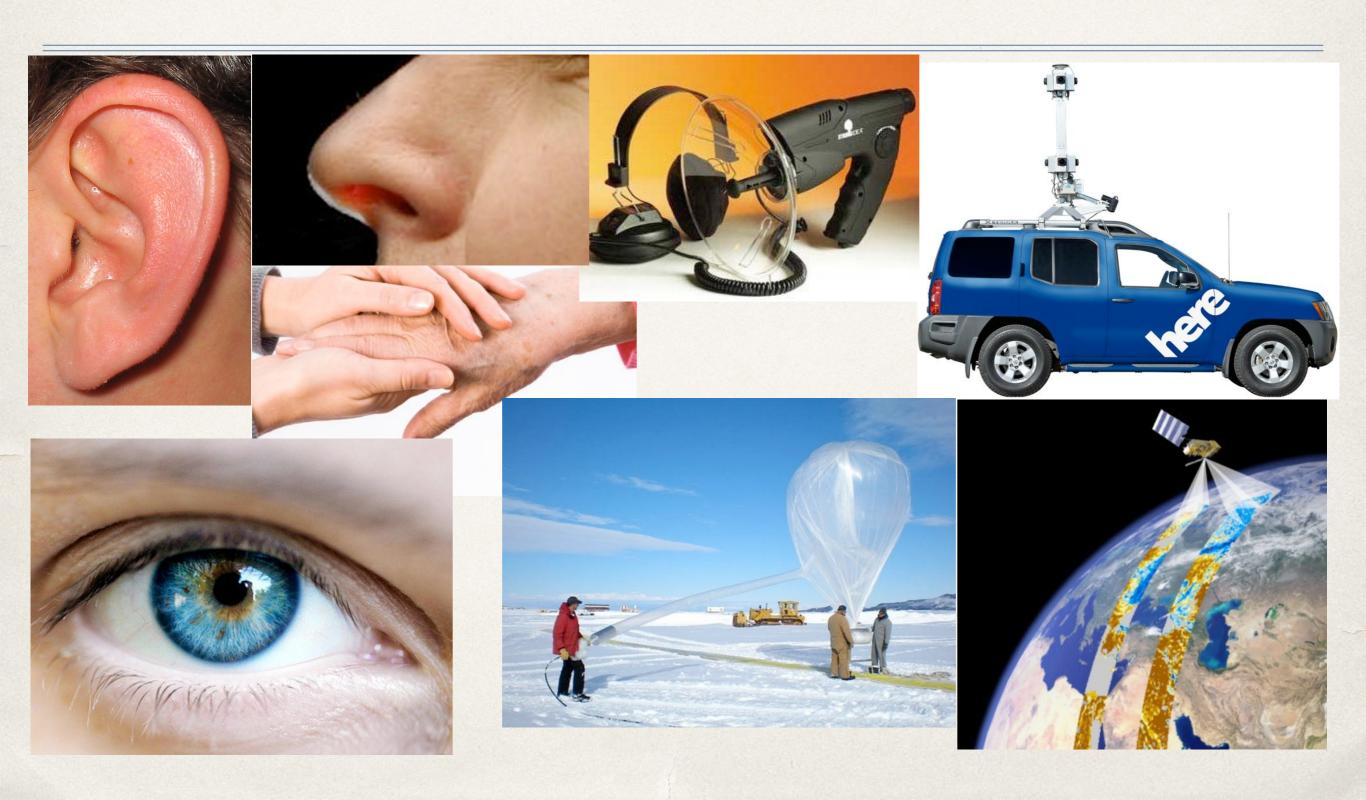


We use data about <u>events</u> to take <u>decisions</u>.



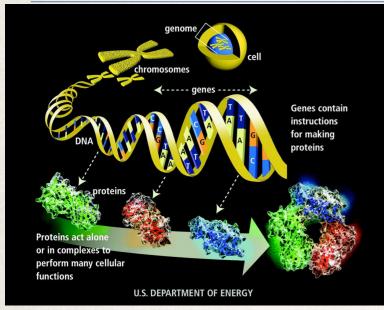
Data sensing? Yes.



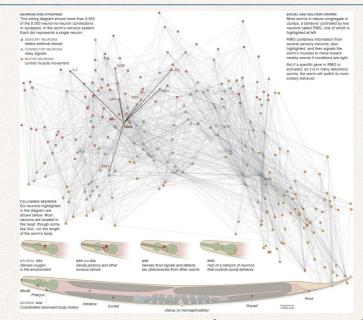


Data storage and processing? Yes.

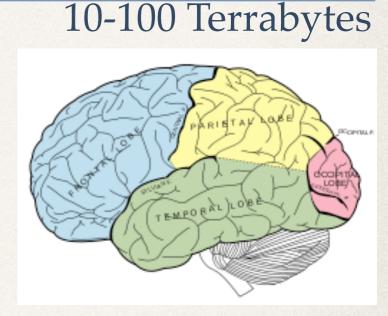
Human brain



Genomes 1kB - 1.5 GB



Worm neural network 0.3MB



In electronic form 1 zettabyte

Raw data is processed and stored

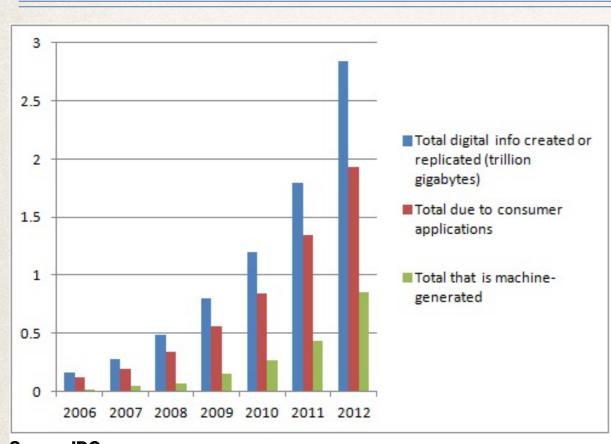


All the books in the world 30-50 Terrabytes



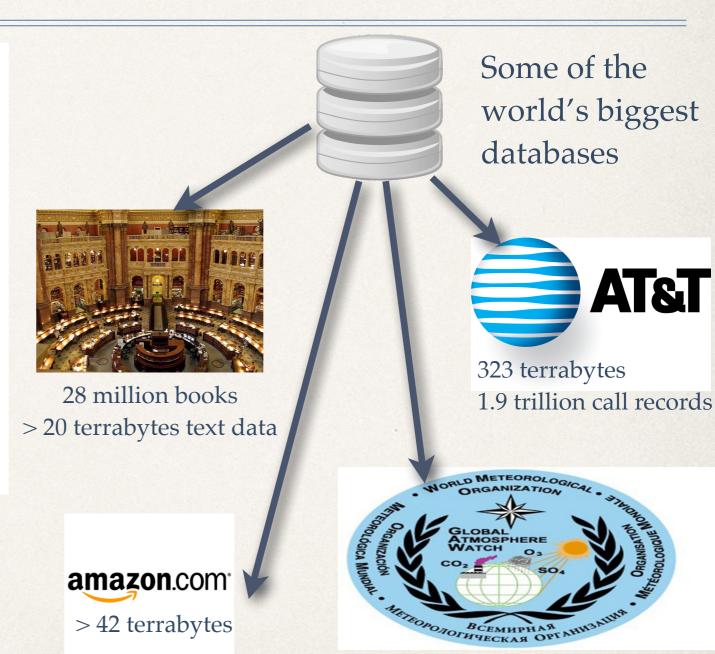
Data storage and processing? Yes.





Source: IDC

Data growth by type



220 terabytes of web data6 petabytes of additional data

Data storage and processing? Yes.



every transaction that occurs is processed (a summary of relevant information is determined) and then electronically stored.

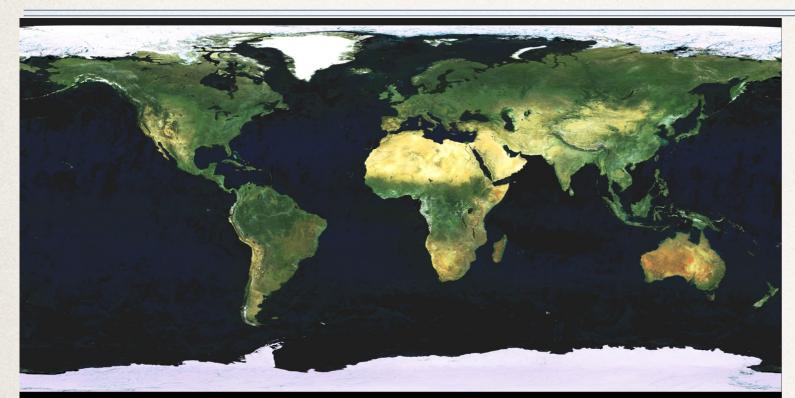
We can now track and record what is happening in the world like never before.

For example, a financial market where...



Data connectivity? Yes.





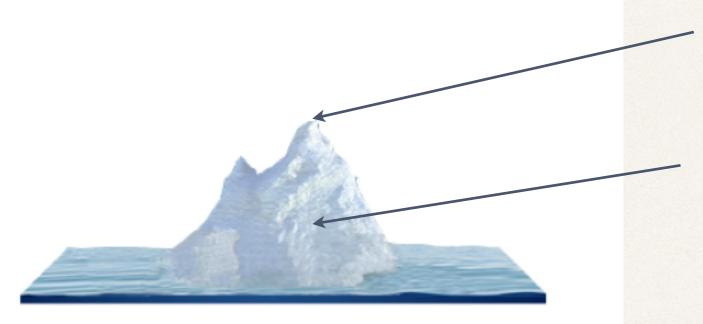
Real space --> cyberspace

Now

Then



Data connectivity? Yes. But just how connected are we?



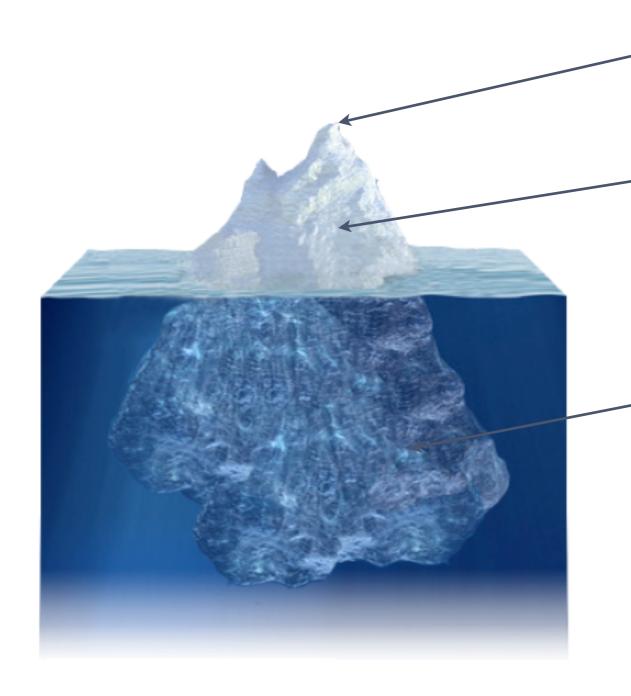
My data: a snowflake

The data we have access to: the tip of the iceberg

Data connectivity? Yes. But is it that great?



Public versus private data



My data: a snowflake

The data we have access to: the tip of the iceberg

The data we don't have access to!

Data search capacity? Yes.





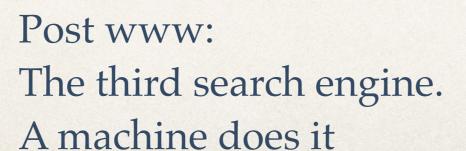
Pre-writing:

The first "search engine". Find the person that knows what you want to know.



Post writing:

The second "search engine" Find the text that contains what you want to know.





Data search capacity? Yes. But just how good is it?



23/04/13 19:55

tery - Google Search

23/04/13 19:45

early victorian educational reforms - Google Search

long rivers

Easy

crhodesstephens@gmail.com

late etruscan pottery

leh Imag

Moi

More ▼ Search tools

About 320,000 results (0.24 seconds)

Etruscan Pottery - The Mysterious **Etruscans**

www.mysteriousetruscans.com/art/pottery.html

Jan 1, 2006 – Most **pottery** found at **Etruscan** burial sites follows very closely on the ... The shapes and motifs of the mid- to **late** 7th century are derived largely ...

Etruscan Art - Metropolitan Museum of Art

www.metmuseum.org/toah/hd/etru/hd etru.htm

Greek **potters** and their works influenced the development of **Etruscan** fine ... source of evidence for artistic achievement during the **Late** Classical and Hellenistic ...

Etruscan art - Wikipedia, the free encyclopedia

en.wikipedia.org/wiki/Etruscan art

The **Etruscans** invented the custom of placing figures on the lid which **later** influenced the Romans to do the same. The Hellenistic period funerary urns were \dots

Impasto (pottery) - Wikipedia, the free encyclopedia





Etruscan - Etruscan Art - HuntFor.com

Web crnodesstephens@gmaff.com Search tools

About 224,000,000 results (0.47 seconds)

List of rivers by length - Wikipedia, the free encyclopedia

en.wikipedia.org/wiki/List_of_rivers_by_length
As a result, the length measurements of many rivers are only approximations. In particular, there has long been disagreement as to whether the Nile or the ...

Definition of length - List of rivers longer than 1000 km

The Longest Rivers in the World - Social Studies for Kids

www.socialstudiesforkids.com/articles/.../longestriversintheworld.htm
Did you know that the longest river in the world is the Nile? Egypt's greatest river is
4,135 miles long! In fact, Africa has two of the ten longest rivers. The Congo ...

Lengths of major rivers, from USGS Water-Science School

ga.water.usgs.gov/edu/**rivers**ofworld.html

Jan 10, 2013 – Ever wonder what rivers are the longest? Look at the graphic below to see our short list of **long rivers**. (It's not so easy to define how long a river ...

Top 9 Longest **Rivers** in the World - UNP

www.unp.me > Chit-Chat > Gapp-Shapp

Aug 23, 2010 - This **long river** can be divided into Ob River and The Irtysh is the major tributary of the Ob. There're several other tributaries for Ob. The water in ...

<u>Top Ten Longest Rivers in the World List - Fun Science Facts for Kids</u> www.sciencekids.co.nz/sciencefacts/topten/longestrivers.html

 $4~{\rm days}$ ago - Longest Rivers in the World. The world features some amazingly long rivers but which are the longest? Check out our list of the top ten longest ...

What are three very long rivers - WikiAnswers

wiki.answers.com > ... > Geography > Bodies of Water > Lakes and Rivers Is this a trick question? Because it can range from 1000 years ago to 100 billion years ago. Which very **long river** in Brazil has its mouth at the Atlantic ocean?

The longest and biggest Rivers of the World

Humans are wonderful at

Top 10 Most Important Rivers In The World - You Tube aren't Semantics, machines aren't

early victorian educational reforms

Image

/ideos

More ▼ Search tools

About 4,220,000 results (0.17 seconds)

Towards Victoria as a Learning Community

www.education.vic.gov.au > Our Department > Strategic Directions
Mar 22, 2013 – Department of **Education** and **Early** Childhood Development ... **Victoria's** Plan for **School** Funding **Reform** • Towards **Victoria** as a Learning ...

Education in **Victoria** - Wikipedia, the free encyclopedia

 $en.wikipedia.org/wiki/ \textbf{Education_in_Victoria}$

Education in **Victoria**, Australia is supervised by the Department of **Education** responsible for the **reform** policy development process and the **early** stages of its ...

Victorian Legislation: a Timeline - The Victorian Web

www.victorianweb.org/history/legistl.html

Dec 20, 2006 – The first **Education** Act did not reach the Statute Books until 1870. 1834 Poor Law Amendment Act. Following the 1832 **Reform** Act, the PLAA ...

Victoria throws education reforms into disarray - The Age

www.theage.com.au > National

Feb 24, 2013 – **Victoria** throws **education reforms** into disarray ... system could be phased in as **early** as next year - and "no school would be worse off".

§25. Public School reform. XIV. Education. Vol. 14. The Victorian ...

www.bartleby.com > ... > The Victorian Age, Part Two > Education
The first steps in a real **reform** of courses of instruction among schools of this type were

taken by the **early Victorian** foundations, chiefly proprietary, such as ...

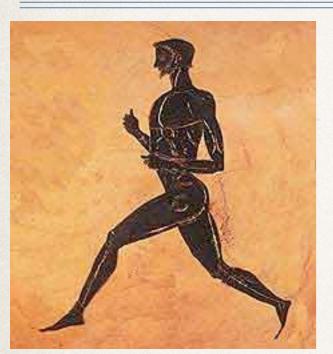
Victorian education reform: Education Act 1870

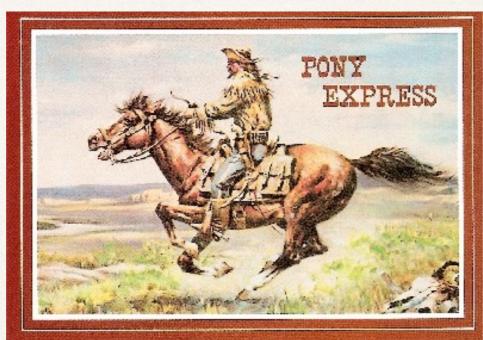
www.architecture.com/.../EducationInAModernWor... - United Kingdom Victorian education reform: Education Act 1870. Perspective view of Harper Street School, New Kent Road, London, 1885. Print Designer: Robert W Edis ...

Doorstop, Melbourne: National Plan for School Improvement ...

Submission on early childhood education reforms - Municipal ...

Data communication speed? Yes, but not like you imagine?

















What's revolutionary? Data purpose? No.



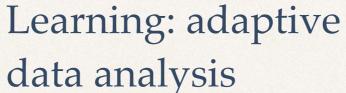
- We have always used data to take decisions
- * There has always been an "evolutionary pressure" in favour of those who can record, process, store and analyse more efficiently and more precisely data in order to make better decisions

Data analysis? Yes.

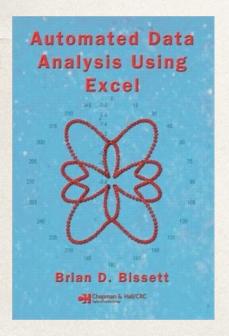




Instinct: Hard-wired data analysis





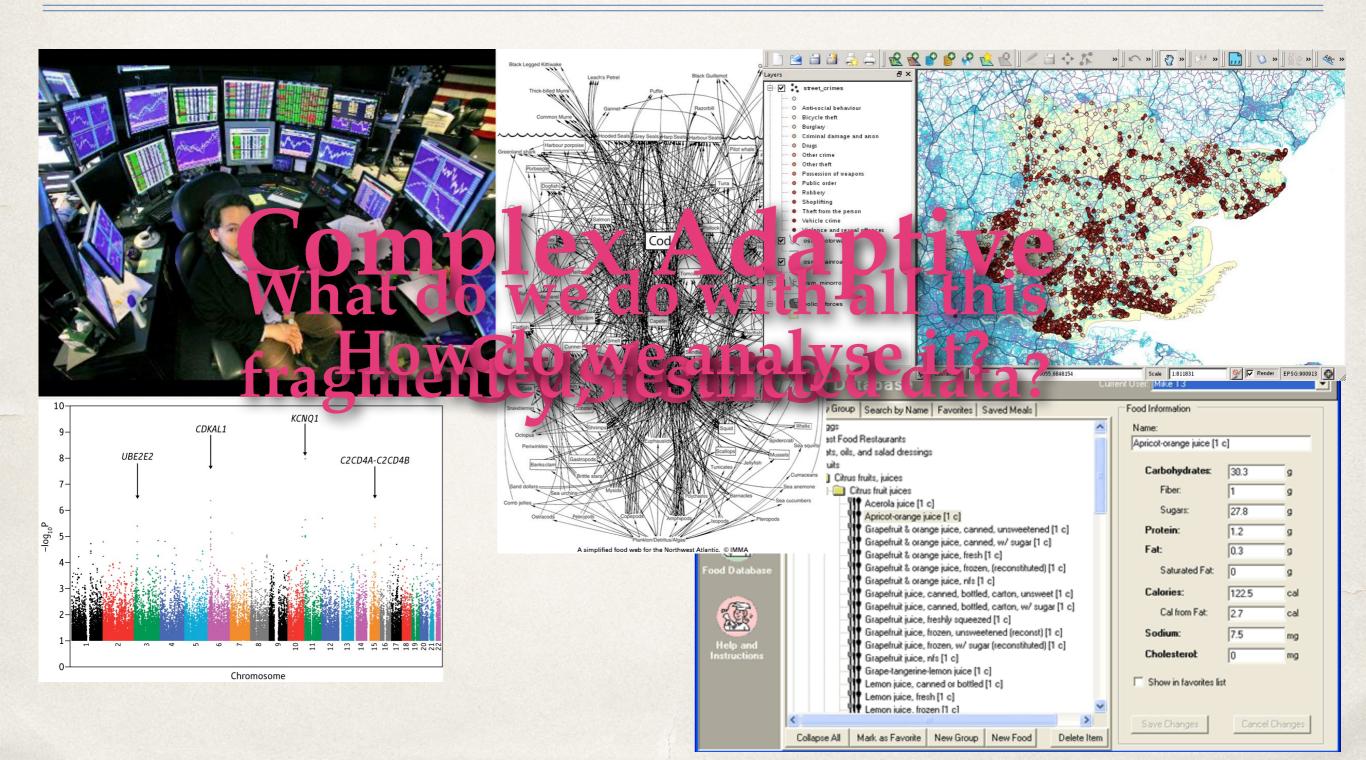


Automated data analysis - data mining. Can consider large volumes of data with large numbers of variables



What does all the data from the data revolution represent?





In Complex Adaptive Systems we need a lot of data because...





you



Imagine what you can say about a city

versus

a crystal as big as a city!

The difference between BIG data and DEEP data

You can say a lot about a Complex Adaptive System and each thing you say depends on a lot of other things

Any observable of a complex system depends on a whole host of other factors

P(A,B,C,D,...; t | a,b,c,d,...; t')

Diabetes Renal failure

Angina

Leukaemia

Obesity Father had diabetes

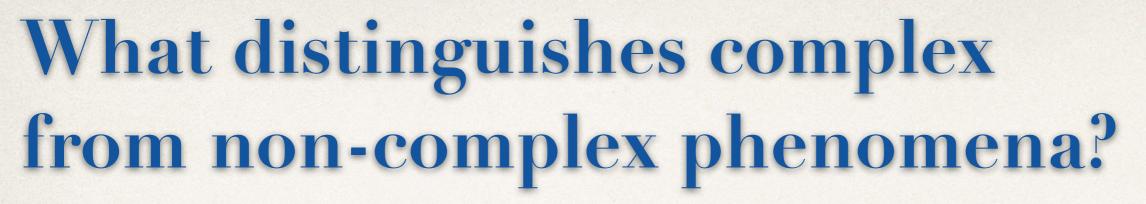
SNP Rs7903146 45 mins exercise

Many effects Many causes per week From the "micro" to the "macro"

Many disciplines



The data revolution is revolutionising our ability to study the immensely rich phenomenology of complex systems and construct more appropriate taxonomies





Structural properties

A "hierarchy" of many different scales

Effective degrees of freedom ("collectivity") that are qualitatively different at different scales

Hierarchies of **building blocks** (modularity)

Interactions that are stronger "intra-block" than "inter-block"

The micro and macro and linked through feedback (fitness, meaning,...)

Functional properties

Systems that are adaptive

A dynamics that depends on many different rules/strategies

Systems that "learn" (feedback from the environment to the system that is used to update the rules)

The micro and macro and linked through feedback (fitness, meaning,...)

More complex behaviour (the "phenotype")

Better described by what they DO than what they ARE



Is complexity a scientific concept?

If it is, then...

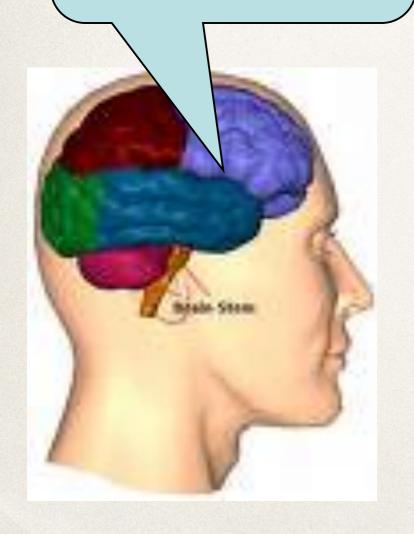
How do we measure it?

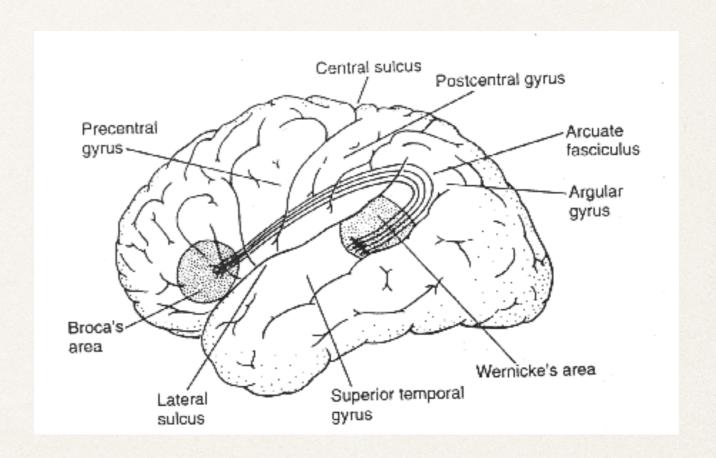
What is a good measuring apparatus...?





To be or not to be that is the question.





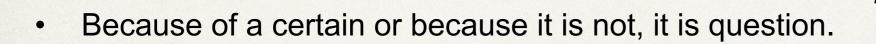
This apparatus is surely capable of measuring complexity. Or maybe not...?



How good is your apparatus?

- To be or not to be that is the question.
- Para ser o no ser que es la pregunta.
- Om te zijn of te zijn niet dat de vraag is.

あるためまたはないため質問である



Because or it is not for the sake of, that having asked and being convinced.

good

good

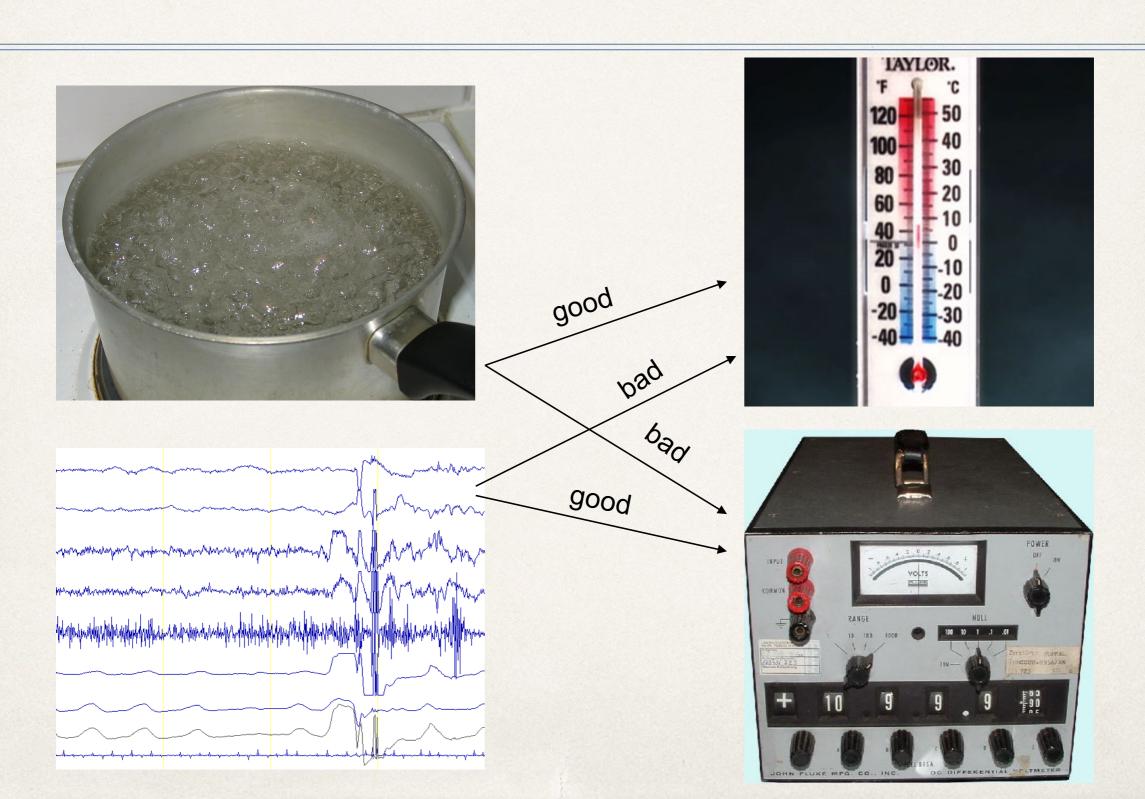
pad

bad

- Being not to be for the sake of, or that that, you ask, are convinced.
- It is that without having for the sake of, or, you ask, are convinced.









Modeling complexity

To make a mathematical model of a dynamical system...

we need a space of states and update rules that tell us how to get from one state to another

Does this represent a Complex System?



$$\mathbf{d}_i(t+\Delta t) = \sum_{j\neq i} \frac{\mathbf{c}_j(t) - \mathbf{c}_i(t)}{|(\mathbf{c}_j(t) - \mathbf{c}_i(t))|} + \sum_{j=1} \frac{\mathbf{v}_j(t)}{|\mathbf{v}_j(t)|} \text{Competition between an effective repulsion and attraction between "particles"}$$

$$\hat{\mathbf{d}}_i(t+\Delta t) = \mathbf{d}_i(t+\Delta t)/|\mathbf{d}_i(t+\Delta t)|$$
 c(t), v(t) – position/direction vectors of a "particle"

$$\mathbf{d}_{i}'(t+\Delta t) = \frac{\hat{\mathbf{d}}_{i}(t+\Delta t) + \omega \mathbf{g}_{i}}{|\hat{\mathbf{d}}_{i}(t+\Delta t) + \omega \mathbf{g}_{i}|}$$

Equation for "charged" particles in an external field g_i

Couzin, I.D., Krause, J., Franks, N.R. & Levin, S.A. (2005) *Nature*, **433**, 513-516.

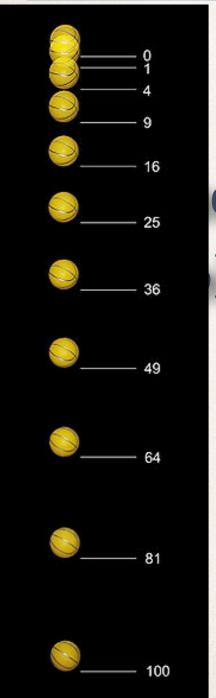
Does this represent a "complex" system?





Moral: It's important to distinguish between a description of complexity and a non-complex description of a phenomenon or behaviour associated with a complex system.

Predictability in physical systems versus Complex Adaptive Systems



Mechanistic

Adaptive

The evolution of function e difference between complex ar is the revolution that allowed le systems is the difference between systems is the difference between systems are sallowed but itself a and a very loss in the parties.

Complexity is a consequence of that revolution.







In biological, economic and social systems, i.e., complex adaptive systems, organisms exhibit a great diversity of **STRATEGIES** (rules/models) that lead to decisions. A strategy can be viewed as a sequence of decisions.

The dynamical state of an individual at t+1 depends not only on the state of the individual at other times t but also on the strategy (update rule) selected at time t, that in turn depends on the rules of others at t. Thus, it is necessary to work in a space of states AND strategies/rules/models – sounds like game theory but

. . .

We don't know what this space is!



Besides, the payoff for a strategy is RELATIVE not absolute. Payoff (fitness) should be an emergent property. Imagine at the beginning of life trying to specify a priori the fitness of a lion or an ant!

Evolved Virtual Creatures

Examples from work in progress

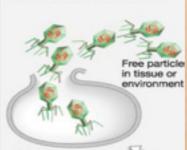












Particles assemble inside host, then burst or bud to exterior.





Predictibilidad en los Sistemas Simples versus los Sistemas Complejos

1) Suelto un objeto de mi mano. ¿Qué pasará?

Cae al suelo 100% Se queda colgado en el aire

0%

2) Dejo dos objetos de distintas masas caen de mis manos. ¿Cuál tocará piso primero?

Lo mas pesado 0% Lo menos pesado 0% Ambos al mismo tiempo 100%

3) Empujo este objeto con mi mano. ¿Qué pasa?

Se mueve 100%

Se queda sin mover 0%

Fenomenología: experiencia cotidiana Las leyes de Newton

¿Qué es predecible? ¿Los seres humanos?



1) No han tomado agua (ningún liquido) en tres días. Alguien te ofrece un litro de agua o una caja de hojuelas. ¿Qué seleccionas?

Agua 100%

Hojuelas 0%

2) Hay un incendio grave en el auditorio y suena la alarma. Yo les invito esperar hasta el final de mi platica o se huyen. ¿Qué haces?

Huyes 100%

Se queda

3) Tienen mucho, mucho hambre. Alguien les ofrece una comida de 1500 calorias para satisfacerles. Pueden seleccionar entre carnitas, enchiladas suizas y frijoles negros; o puro apio (7.5kg). ¿Qué seleccionas?

Carnitas etc. 100%

Apio

0%

¿Qué es predecible? ¿Los seres humanos?



4) No han tomado agua (ningún liquido) en tres días. Alguien te ofrece un litro de Coca-cola o un litro de Pepsi. ¿Qué seleccionas?

Coca cola 70%

Pepsi 30%

5) Hay un incendio grave en el auditorio y suena la alarma. Llegaste a la salida pero notas alguien quien no conoces atrapado. Regresas para tratar de ayudarles arriesgando tu propia vida o sigues corriendo?

Si regresas 50%

No regresas 50%

6) Tienen mucho, mucho hambre. Alguien les ofrece una comida de 1500 calorias para satisfacerles. Pueden seleccionar entre carnitas, enchiladas suizas y frijoles negros; o barbacoa, chicharrón y arroz ¿Qué seleccionas?

Carnitas etc. 50%

Barbacoa etc. 50%

Conclusions:



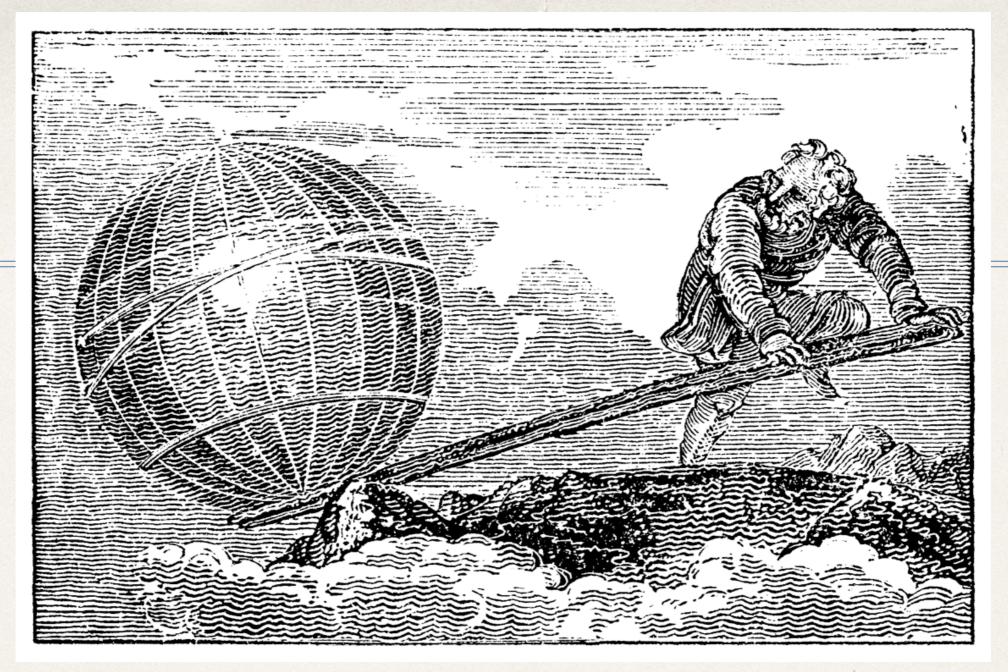
- * All science is "data science" from its beginnings to the present day. There is no science without data.
- * Because of universality physical systems are relatively phenomenologically poor (**big** data but not **deep**!) and therefore need relatively little (shallow) data (CERN, LIGO, etc. notwithstanding)
- * Phenomena at one scale in the physical sciences is shielded from the rest ("effective theories") and that's why physics has been so successful
- Complex Adaptive Systems are phenomenologically deep and need a lot of data to describe them...

Conclusions: The data revolution

- * We are generating 1 Zettabyte of data per year. That's about 1 Terrabyte per person per year. That's more than a million books!
 - * Humans can't use or analyse all of that data
 - Should we just dump it or ignore it?
 - * There is a huge potential for good (or ill) in much of the data
 - Who should have access to it?
 - Who should decide how its to be used?
- * The collection, use and abuse of this data will probably be the most significant factor in our history over the next 100 years

Conclusions: Complex Adaptive Systems

- * We don't have adequate conceptual or theoretical frameworks in which to understand complex adaptive systems or complexity
 - Physical systems "are", while complex (adaptive) systems "do"
 - * Physical systems are described by few relevant variables, for complex adaptive systems there are many that range from the micro to the macro
- * Good science starts with phenomenology and taxonomy before moving on to theory we have many "Brahes" but we need more "Keplers" and less "Newtons"
- Basically all the data generated in the data revolution is "non-scientific" and is associated with complex adaptive systems
- The traditional modeling frameworks of the physical sciences are much less useful in the Complex Sciences
- * Data mining/machine learning/Deep learning/... are just methodological tools to help us be better "Keplers". They offer the best way to attack this data. Its also the appropriate way to develop a better phenomenological and taxonomic understanding of complex adaptive systems



δῶς μοι πᾶ στῶ καὶ τὰν γᾶν κινάσω Give me a place to stand on and I'll move the earth

Give me enough data and I'll predict anything