To boldly go where no
man has gone before

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

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

MexiCOPAS
Universidad de Guanajuato 02/05/2017

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…

# The principal purpose of living systems and the principal purpose of science is to…

# Predict

# The principal purpose of living systems and the principal purpose of science is to…

# Predict

for

# The principal purpose of living systems and the principal purpose of science is to…

# Predict

for

# Decision making

# Predict

for

# Decision making

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

# How we do science in a nutshell…

## The traditional approach

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## The traditional approach

- **The Scientific method:** Systematic observation, measurement, and experiment, and the formulation, testing, and modification of hypotheses

- **Phenomenology** - a body of knowledge that relates empirical observations of phenomena to each other, in a way that is *consistent* with fundamental theory, 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.

  - Examples: Medicine, astronomy, chemistry, biology, physics,...

- **Scientific law** - when a particular phenomenon always occurs if certain conditions are present

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DATA

# And the "modern" approach? Data Science —> Data Mining

"… 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 centuries:

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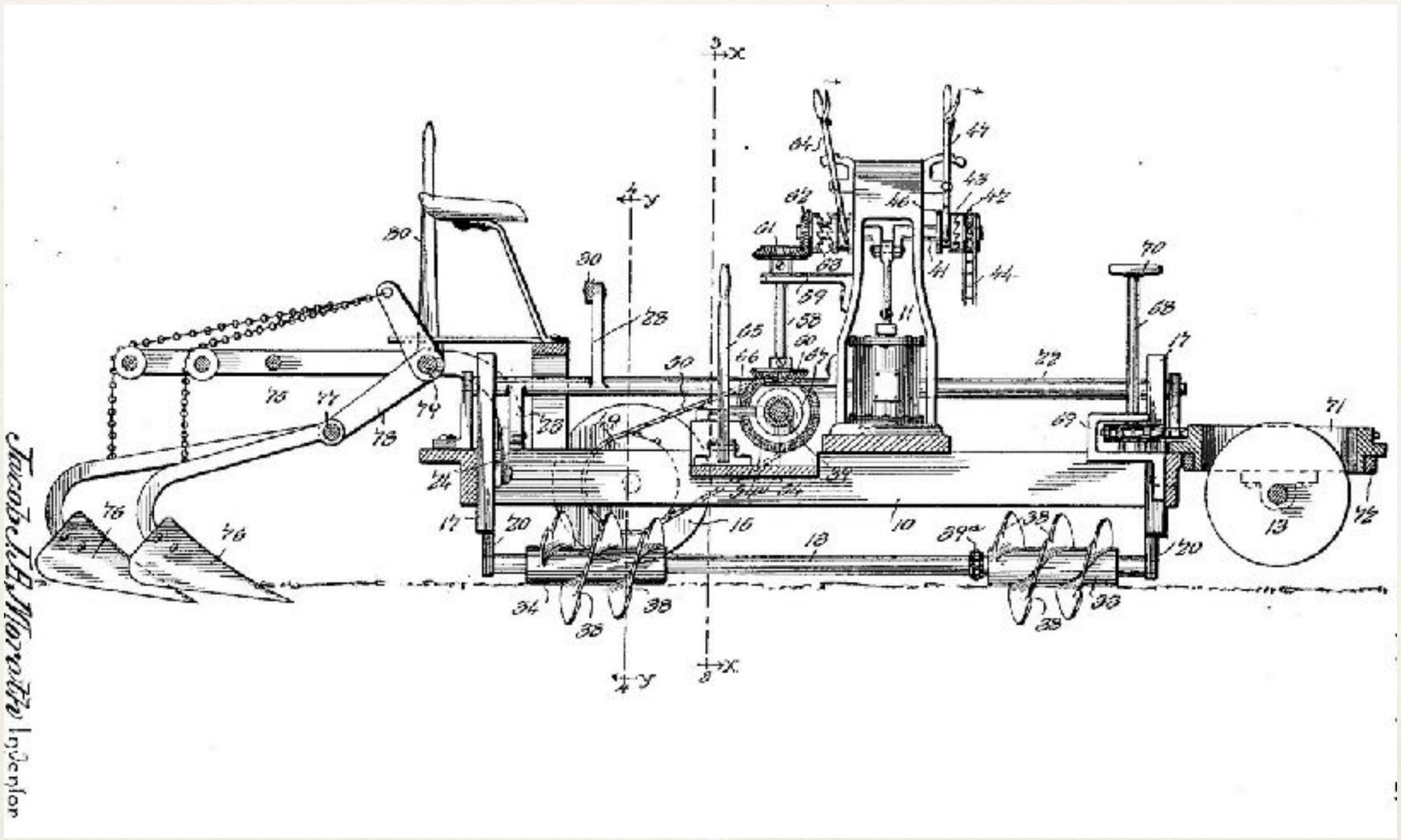

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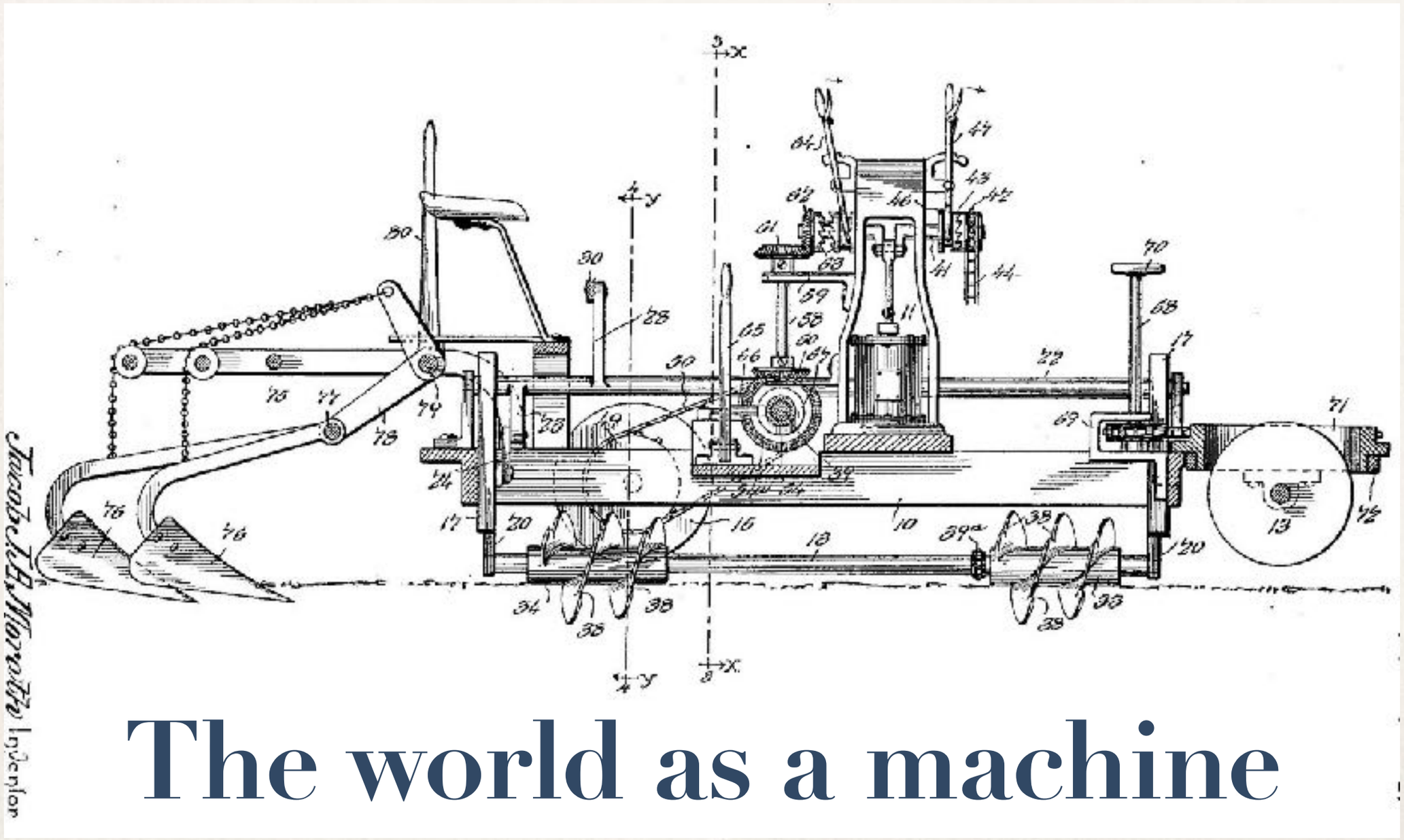


# The world as a machine

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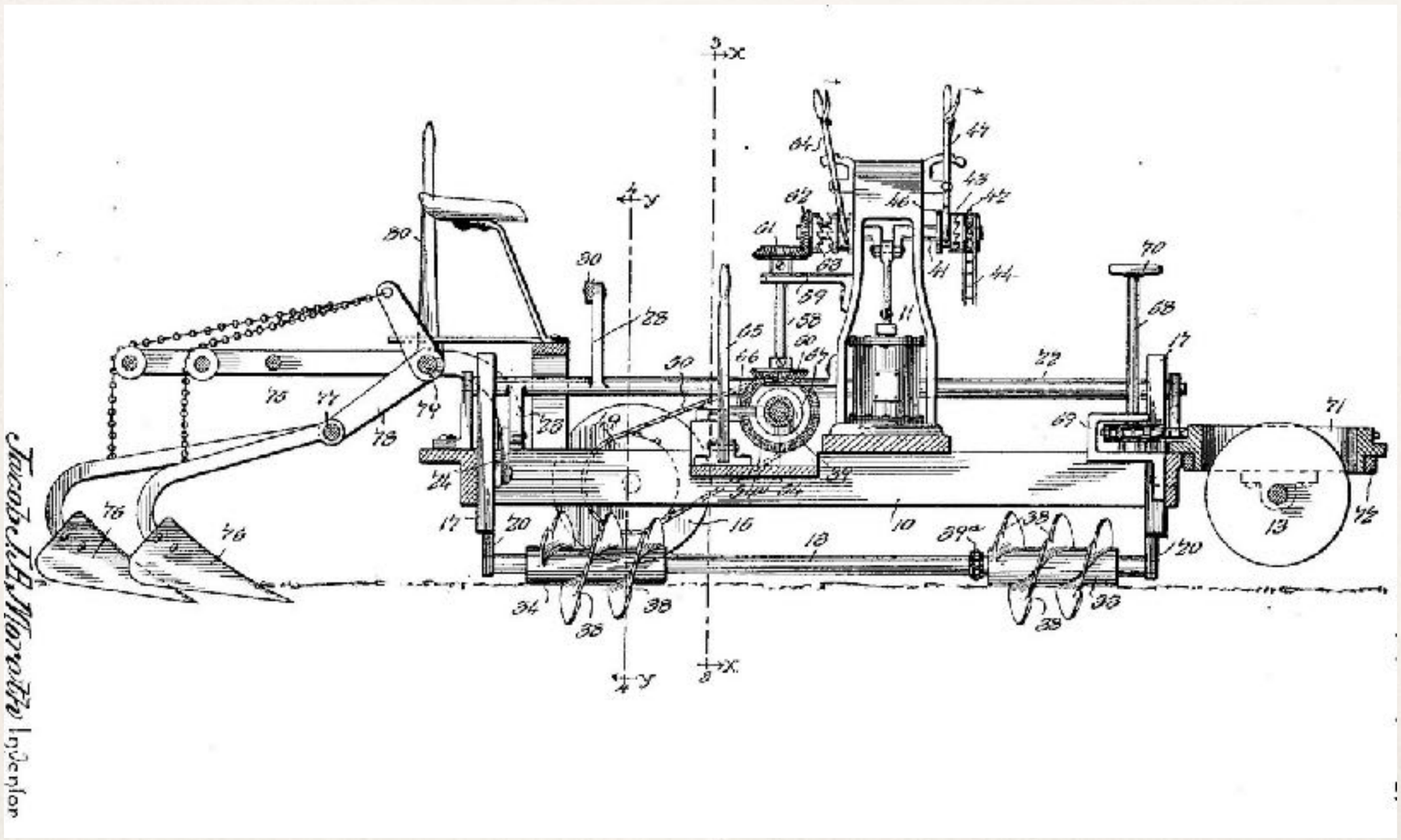

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**We all obey the law!**

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## In fact...

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# The worldview of the last 3 centuries:

## In fact...

# The worldview of the last 3 centuries:

## In fact...

## we are slaves of the law

# Universality

## We're all equal under the law

# Universality

## We're all equal under the law

# But in physics and chemistry...

# Universality

## We're all equal under the law

# Universality

## We're all equal under the law

## there's really not a lot to say

# Universality

## We're all equal under the law

# Universality

## We're all equal under the law

**once you've seen one perfect gas you've seen them all!**

# Universality

## We're all equal under the law

# Universality

## We're all equal under the law

## At all times and in all places

# Universality

## We're all equal under the law

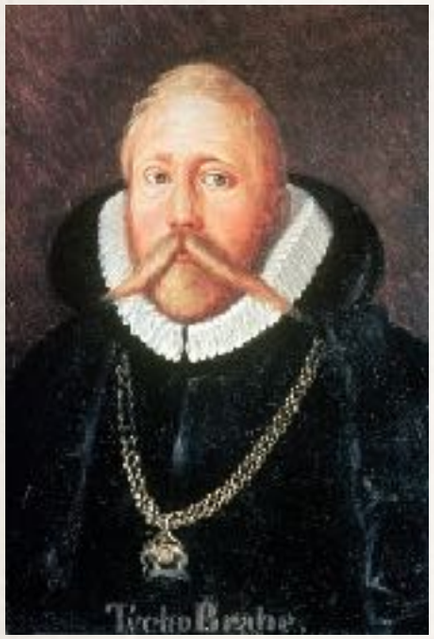
# Universality

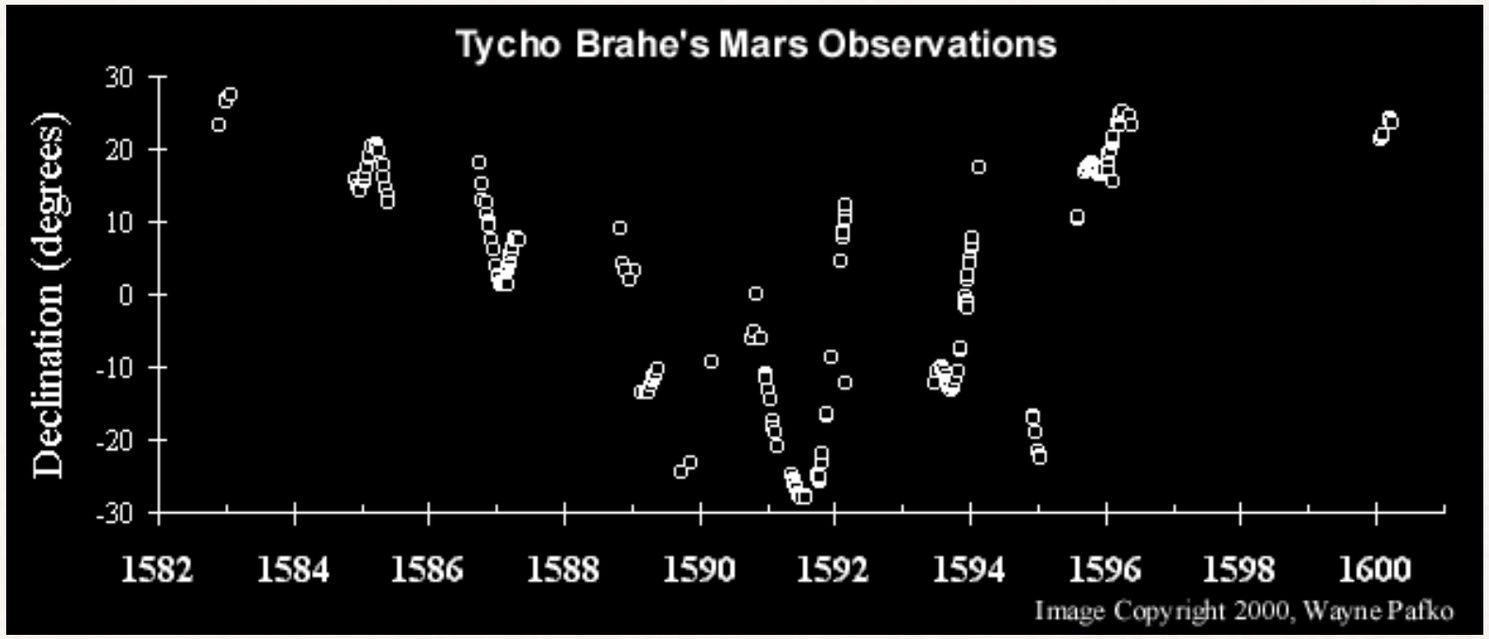
## We're all equal under the law

**In general, you don't need that much data**

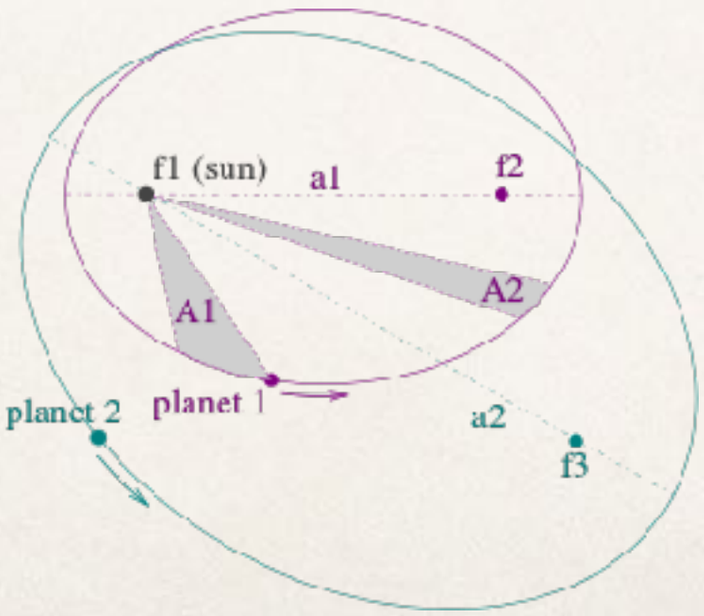
# Isn't all Science Data Science?

## Data —> Phenomenology —> Taxonomy —> Theory






Data




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?

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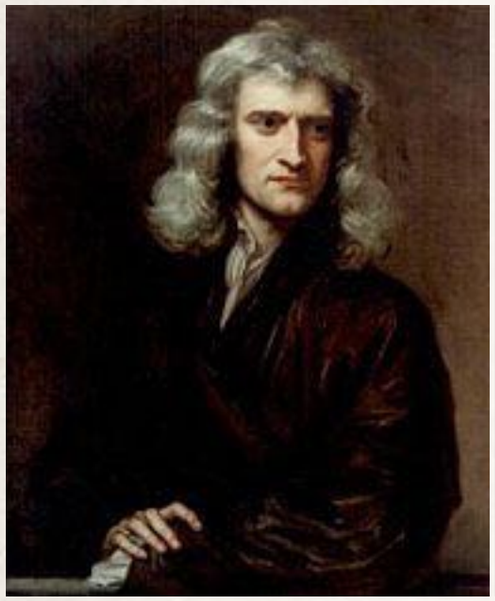

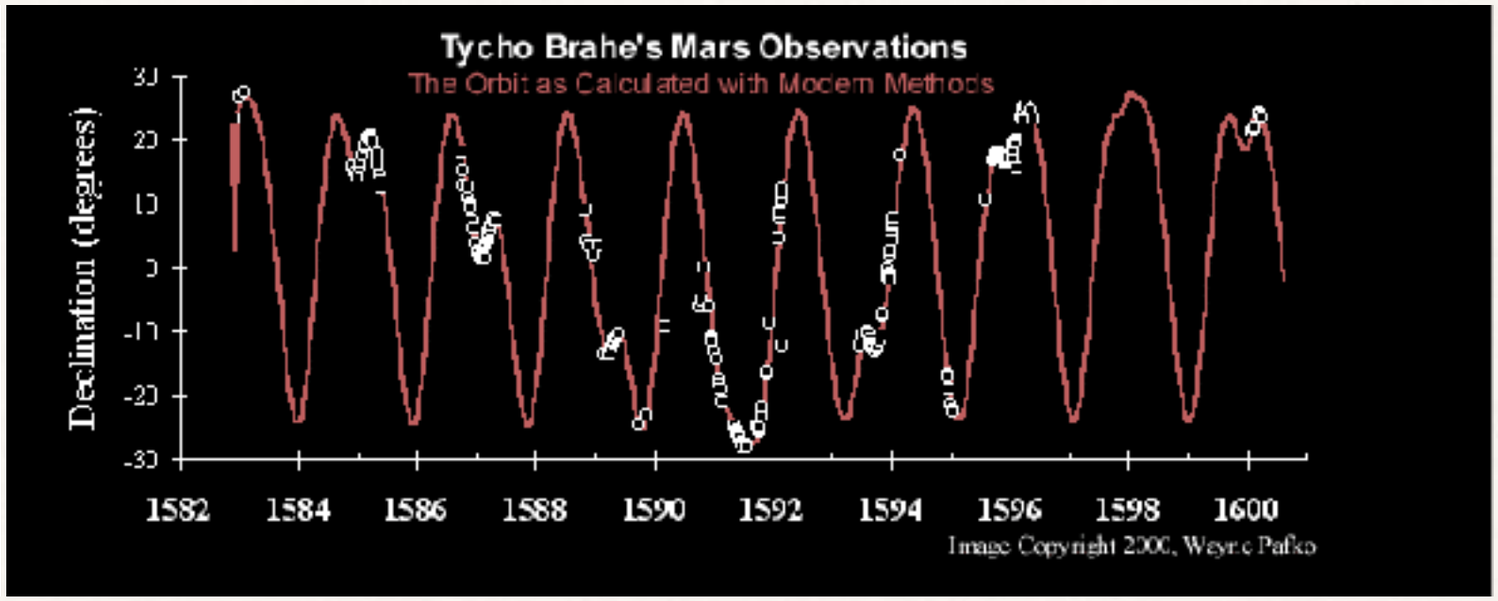


### Theory

$F = ma$

$F = GMm / r^2$

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 **inferred** 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

Camille Kubie, Estuary, 2014

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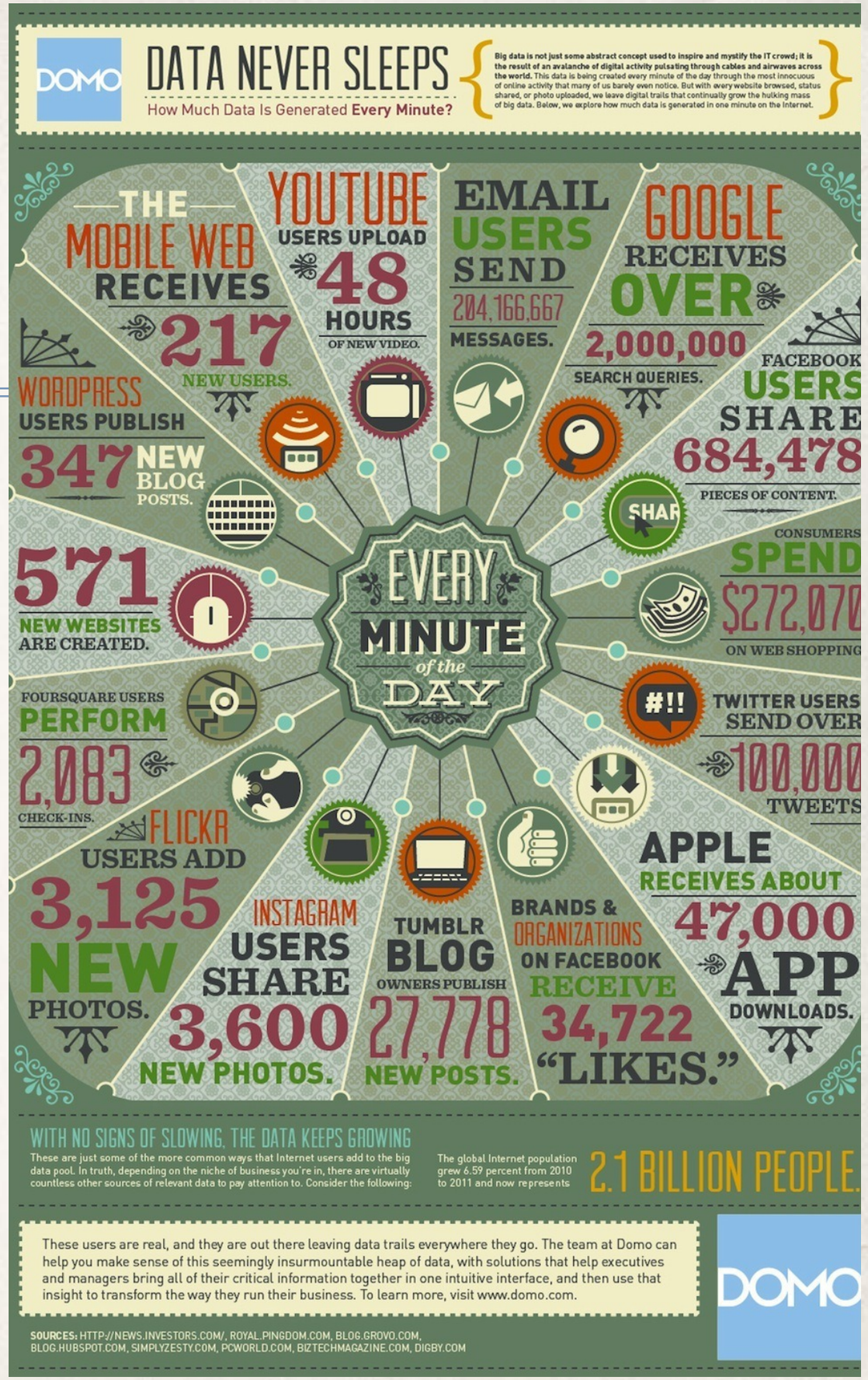
There's been a data revolution...

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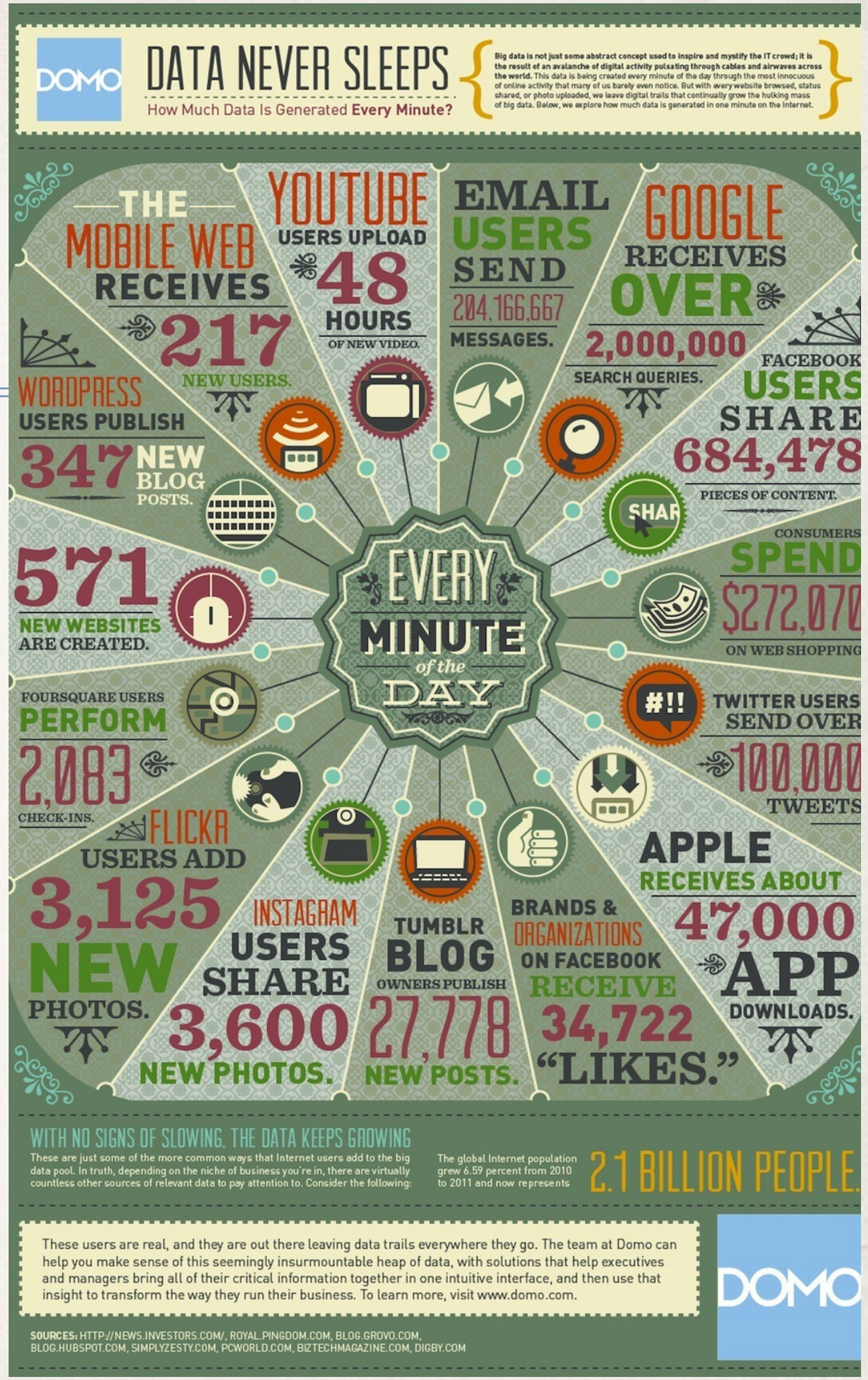
There's been a data revolution...

But just what's revolutionary?

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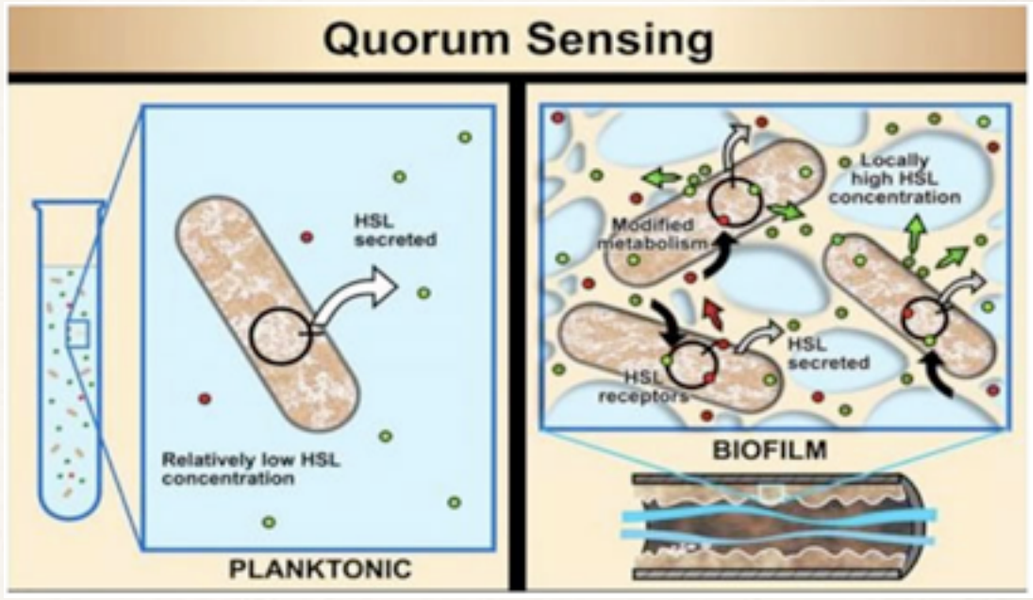
# What's revolutionary?

## Data types? No.

**Raw data:**
Chemical
Electromagnetic
Acoustic...

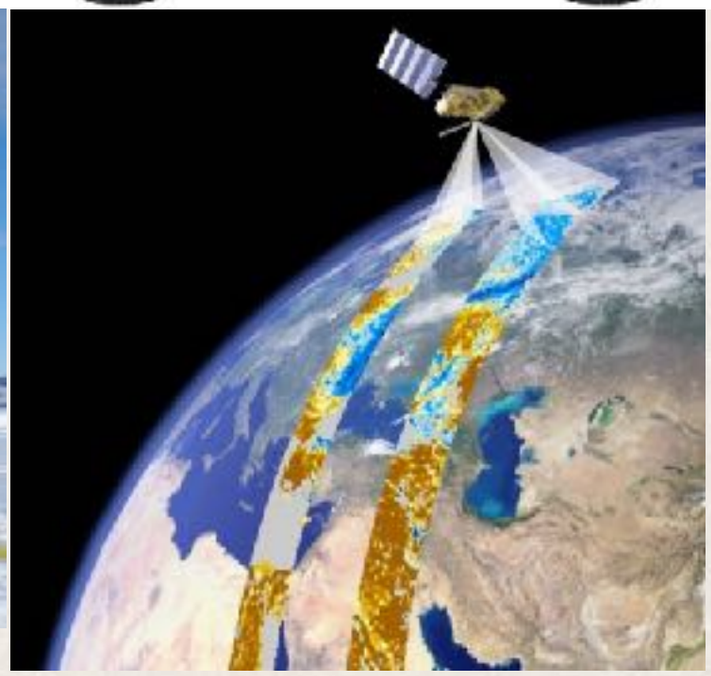
as functions of space and time tell us what is going on in the world.



We use data about ***events***

to take ***decisions.***

# Data sensing?



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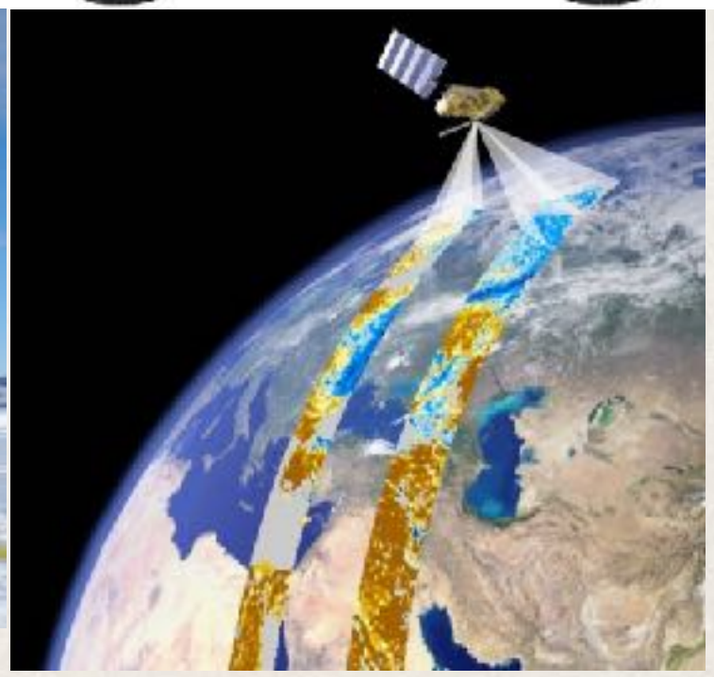
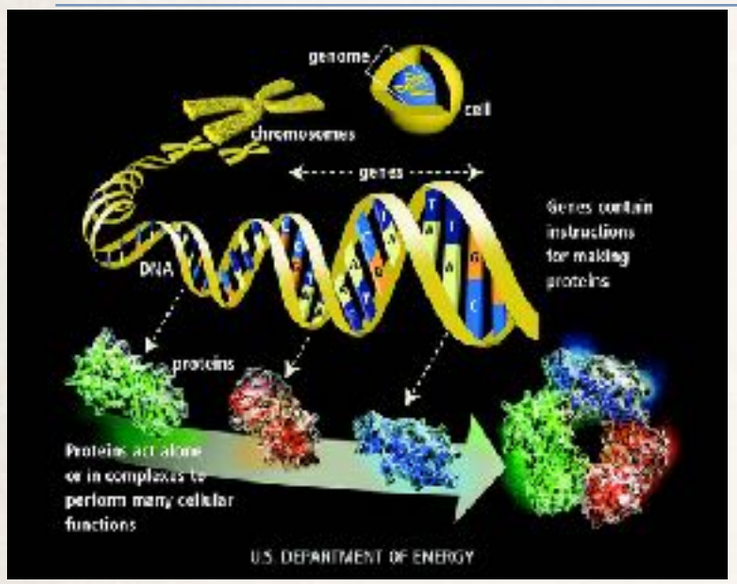
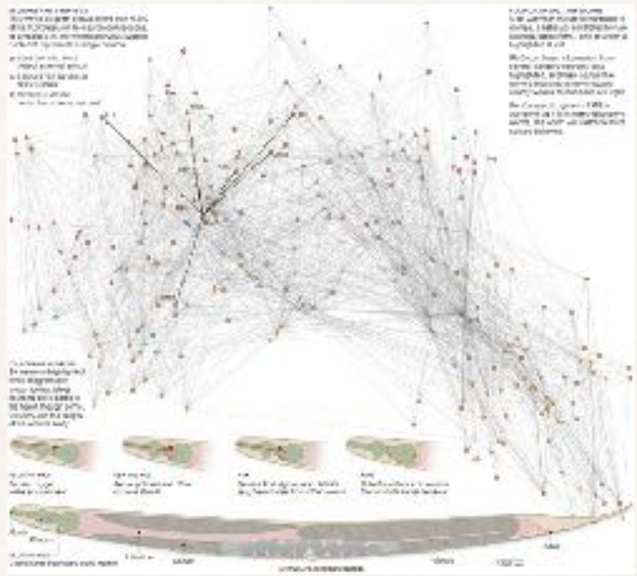


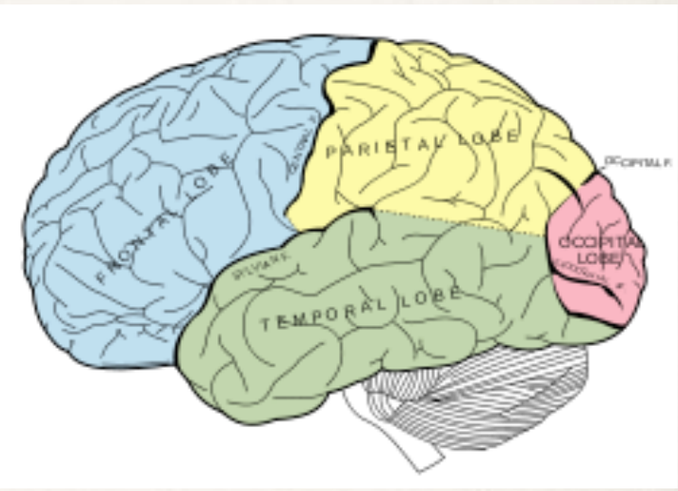
# Data storage and processing?

Human brain

10-100 Terrabytes






Genomes 1kB - 1.5 GB

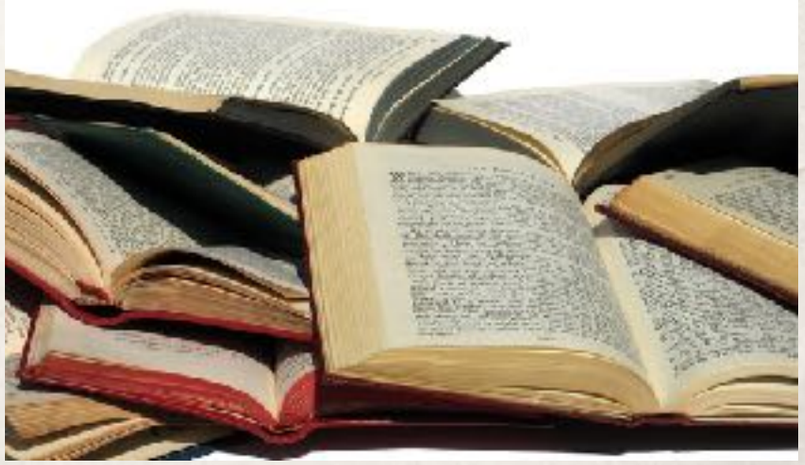
Worm neural network 0.3MB

In electronic form 1 zettabyte

***Raw data is processed and stored***

All the books in the world

30-50 Terrabytes



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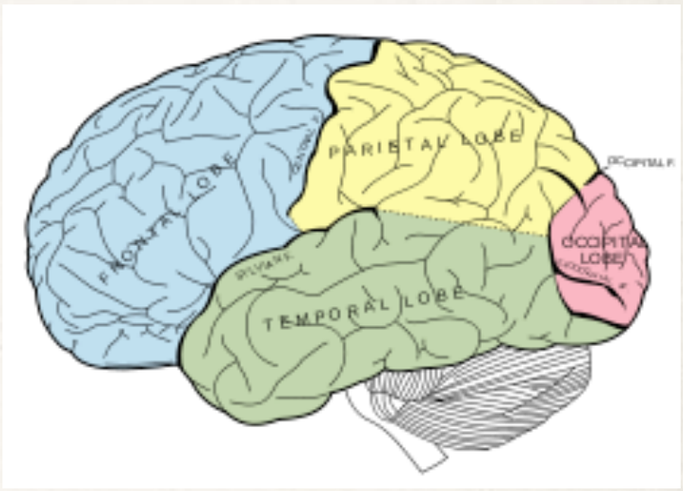


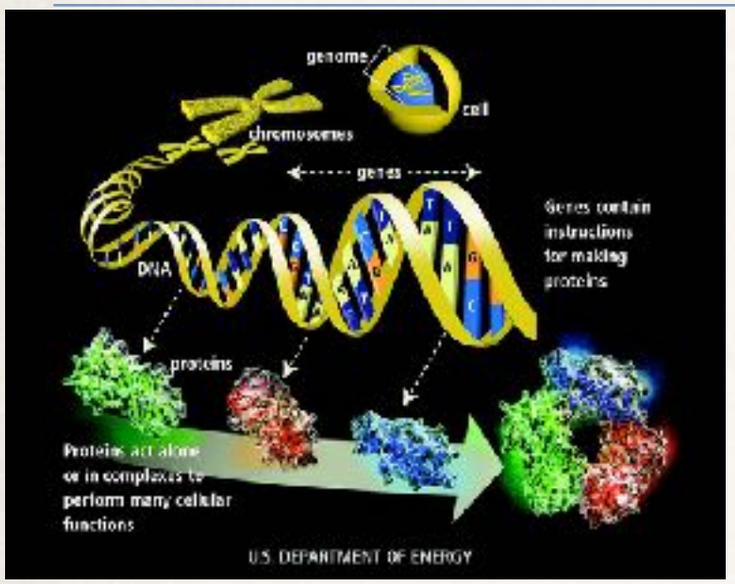


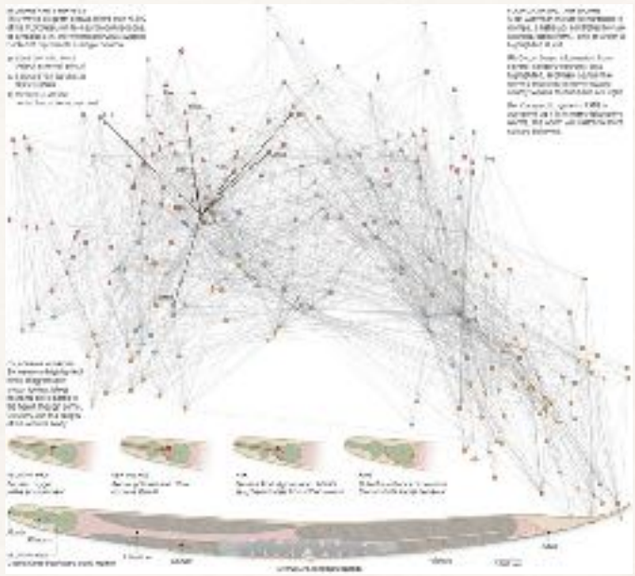

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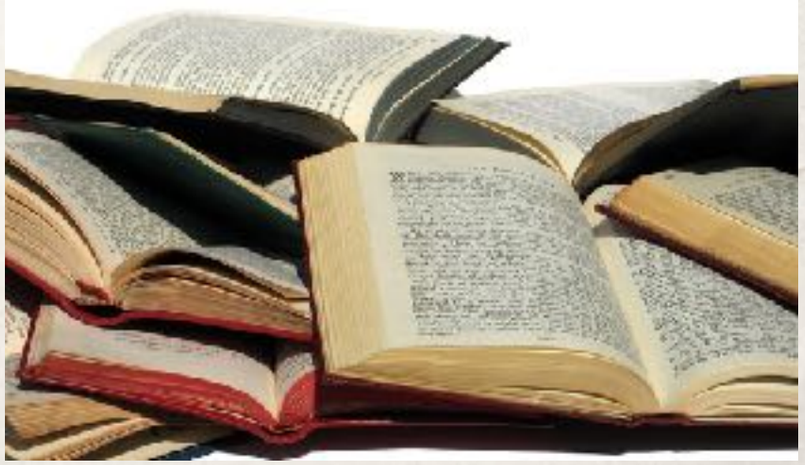

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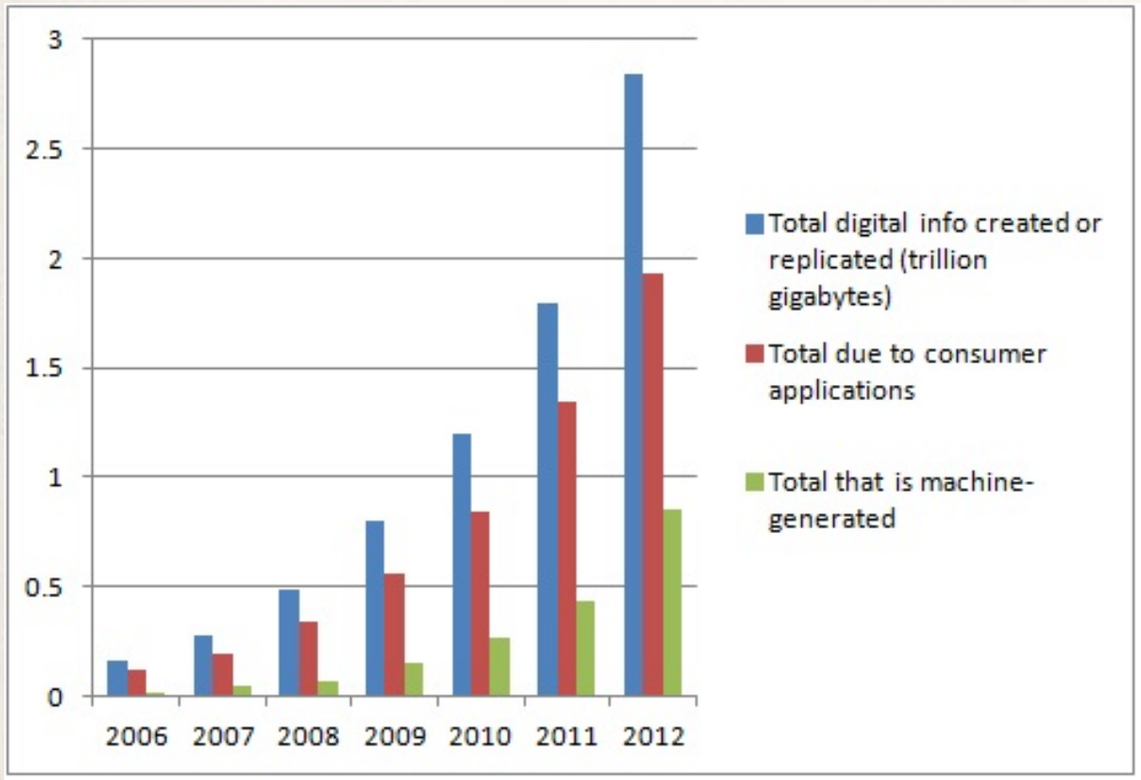



**Source: IDC**

Data growth by type

28 million books
> 20 terrabytes text data

Some of the world's biggest databases

323 terrabytes
1.9 trillion call records

amazon.com

> 42 terrabytes

220 terabytes of web data
6 petabytes of additional data

# What's revolutionary?

## Data storage and processing? Yes.

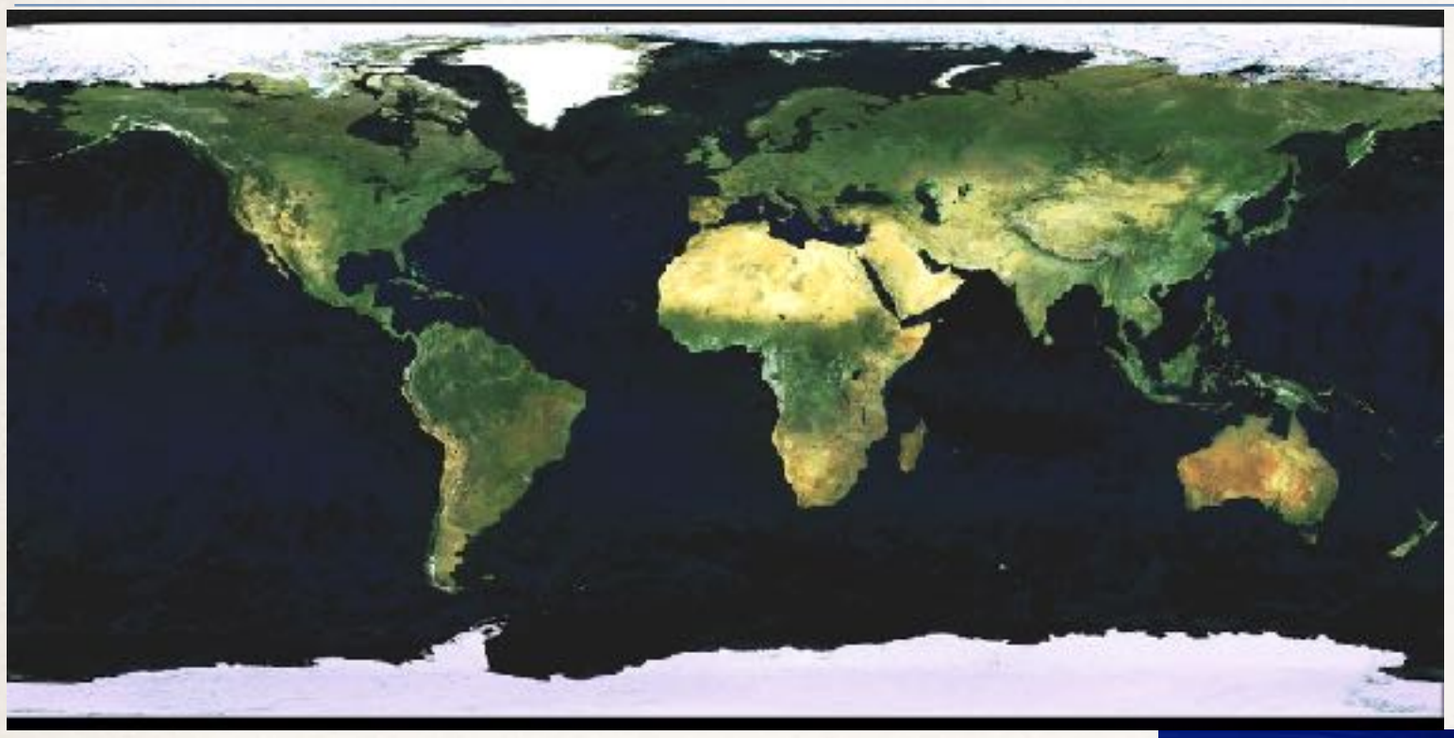
We can now track and record what is happening in the world like never before.

For example, a financial market where...

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

# What's revolutionary?

## Data connectivity? Yes.



Real space --> cyberspace

Then

Now

# Data connectivity?

# Data connectivity? Yes.

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

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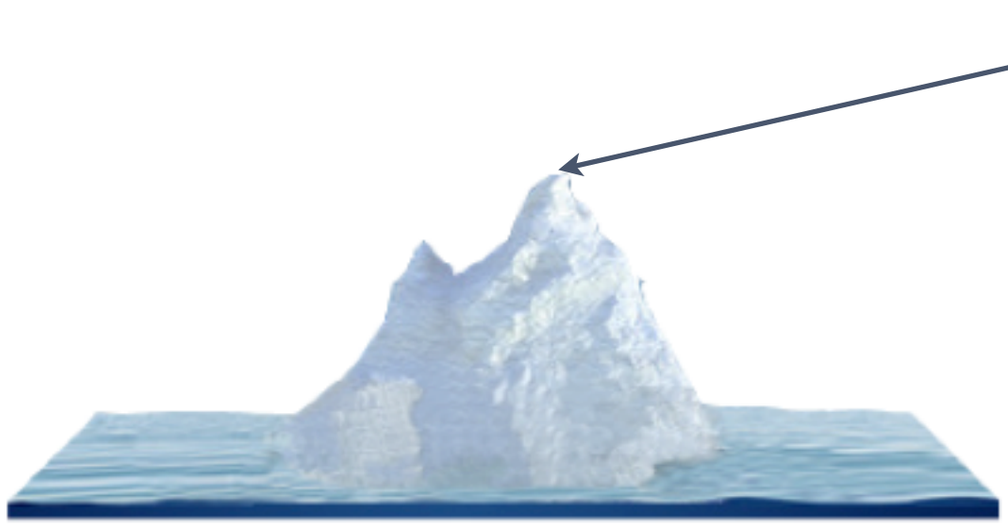

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# But just how connected are we?

My data:
a snowflake

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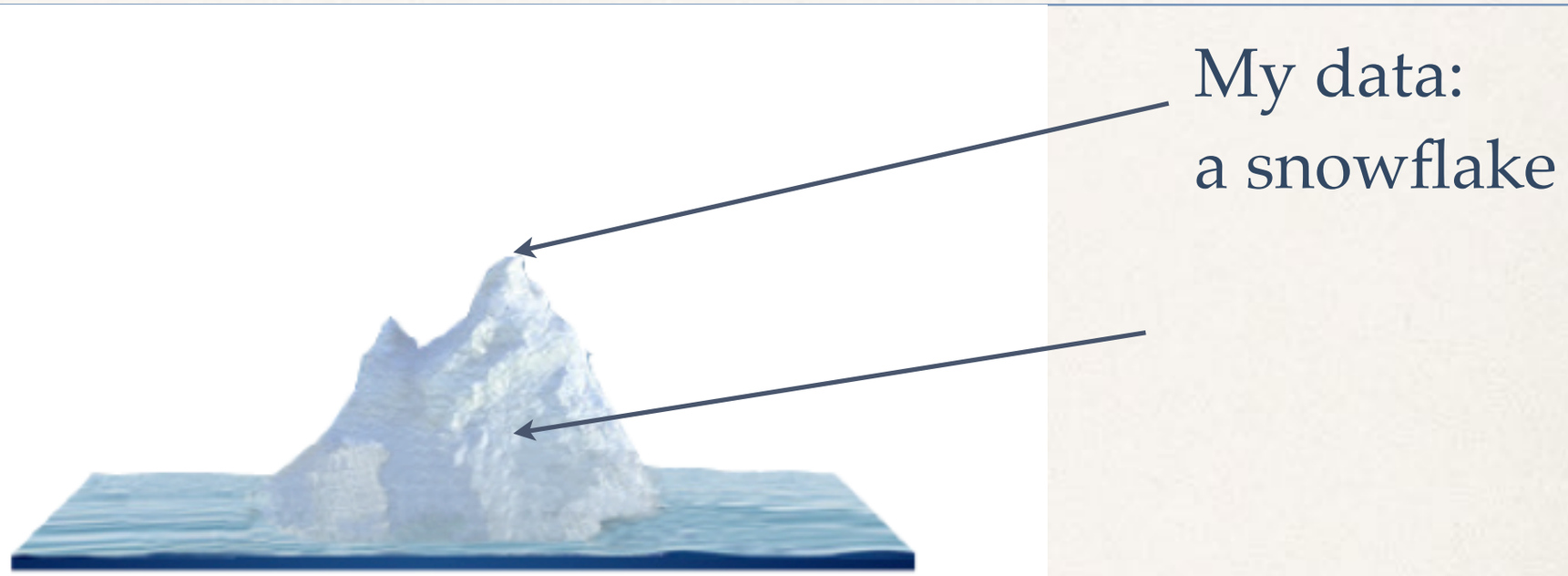

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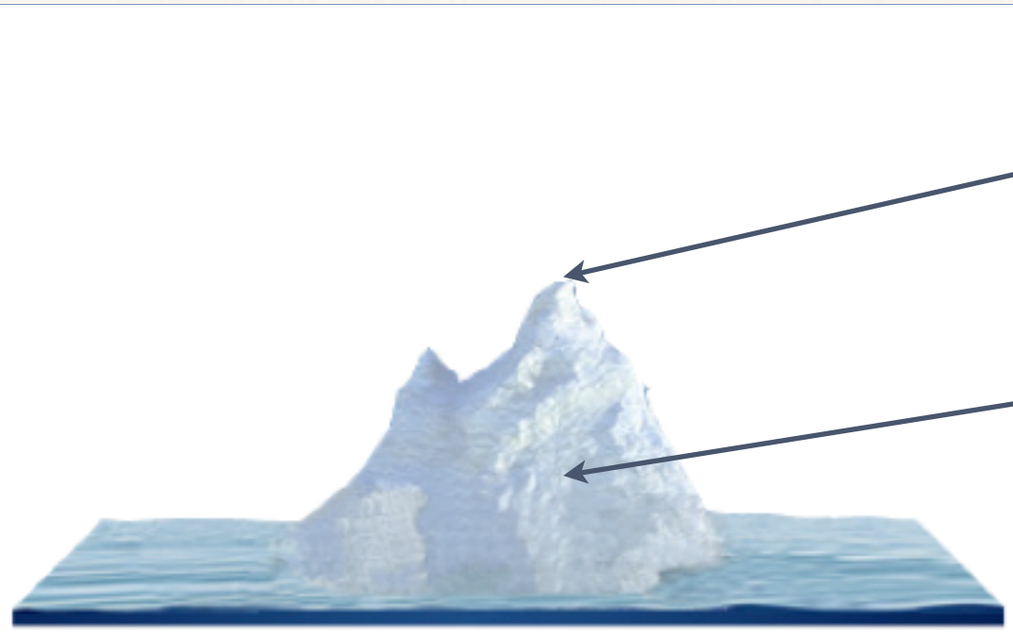
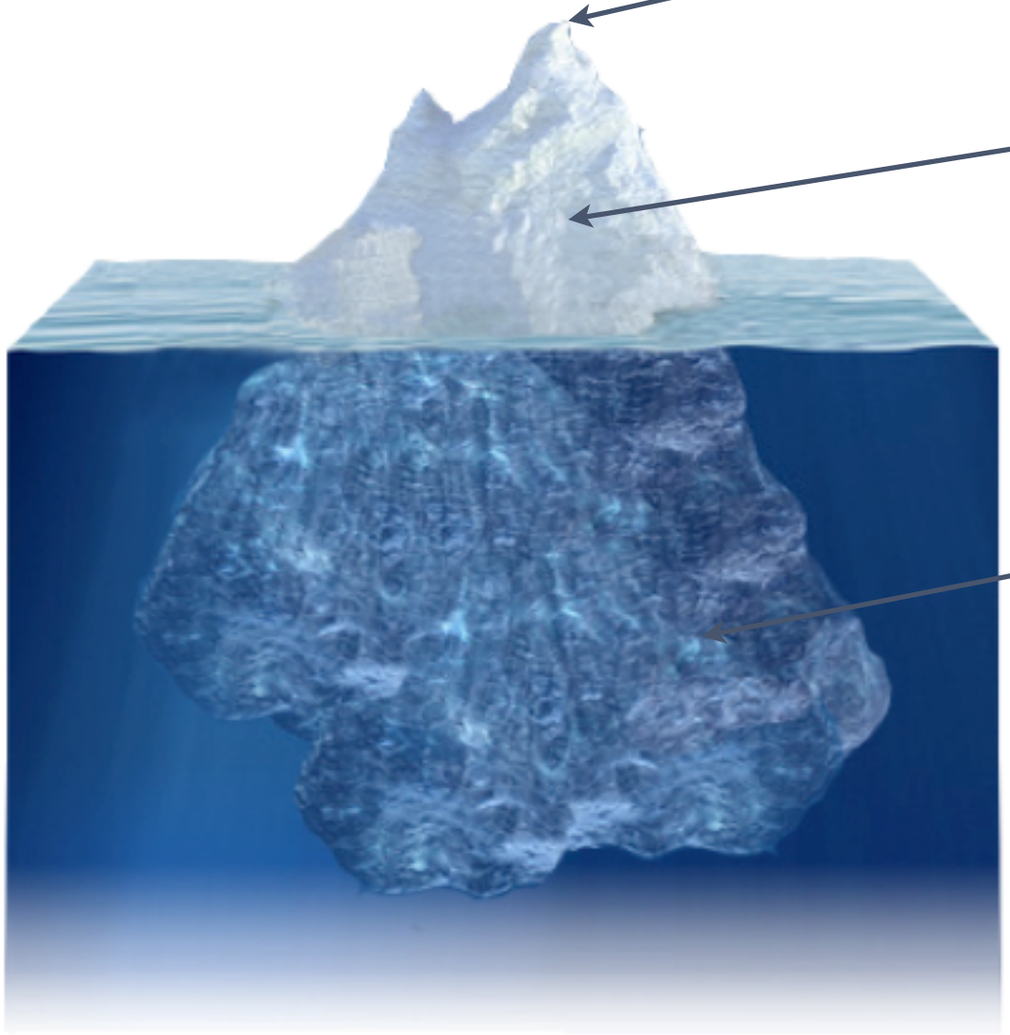


My data:
a snowflake

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!

# What's revolutionary?

## 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.

Post www:
The third search engine.
A machine does it

# Data search capacity?

# Data search capacity? Yes.

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

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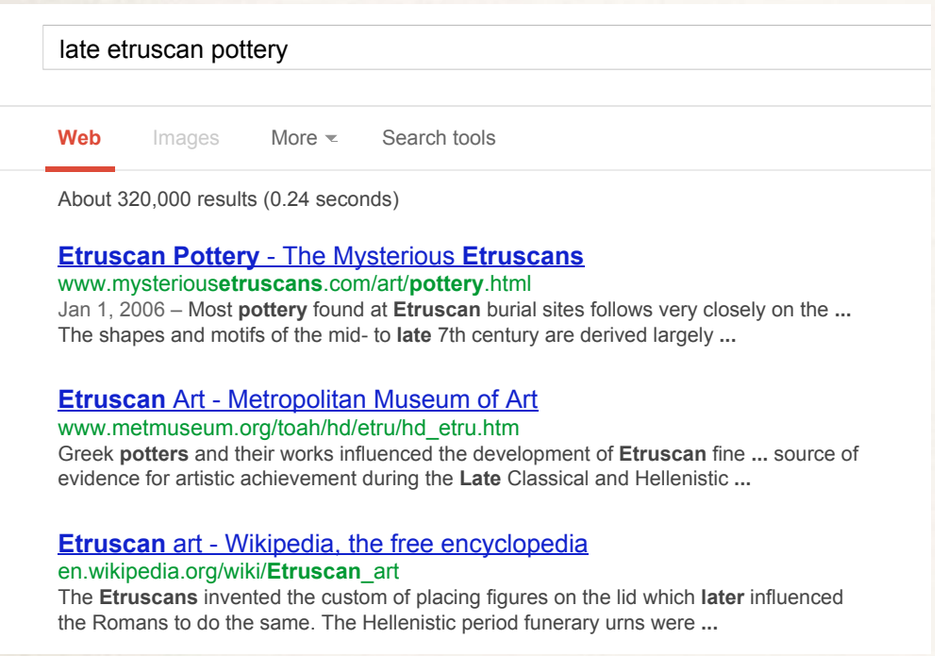

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***It's fast but not clever!***

Humans are wonderful at semantics, machines aren't

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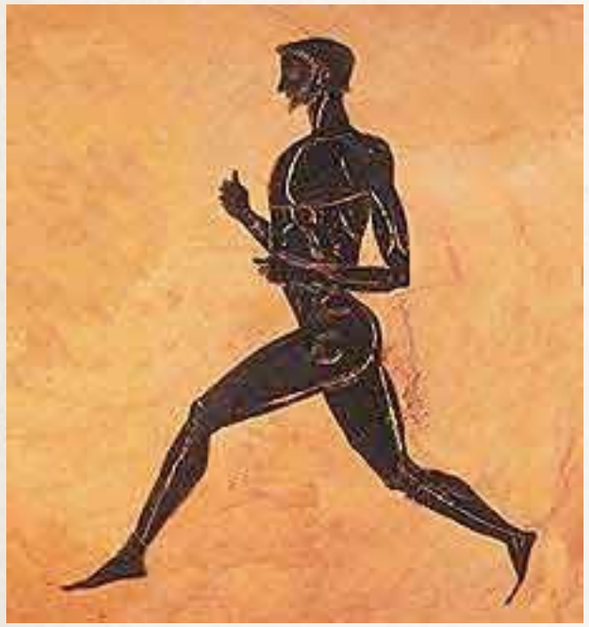
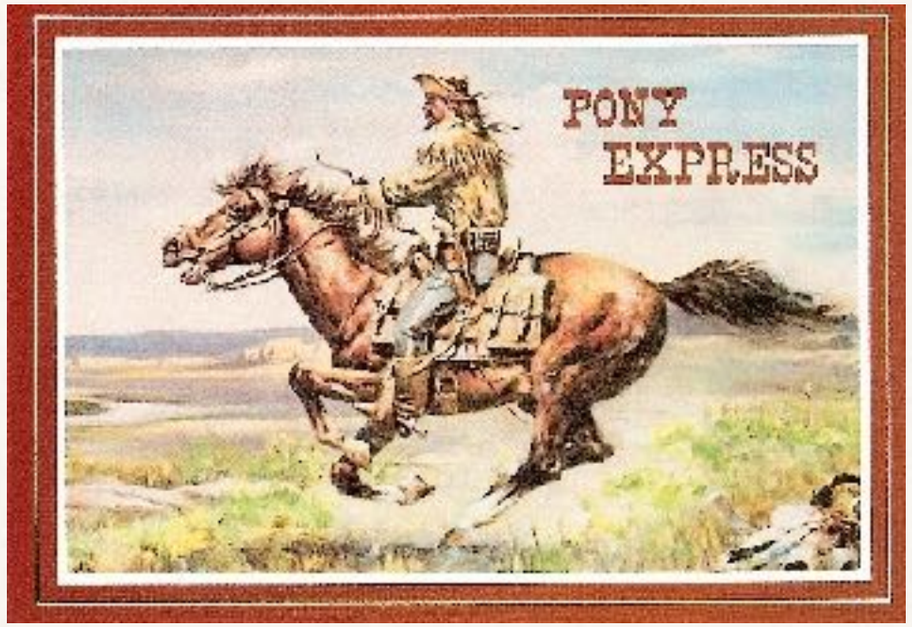
## Data communication speed? Yes, but not like you imagine?





# What's revolutionary?

## Data purpose? No.

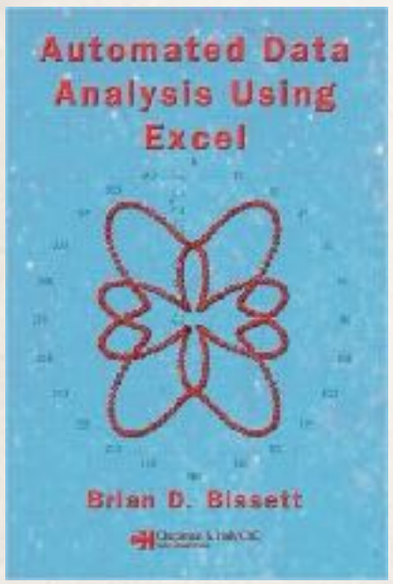
- We have always used data to take decisions

- 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?

Instinct: Hard-wired data analysis

Learning: adaptive data analysis

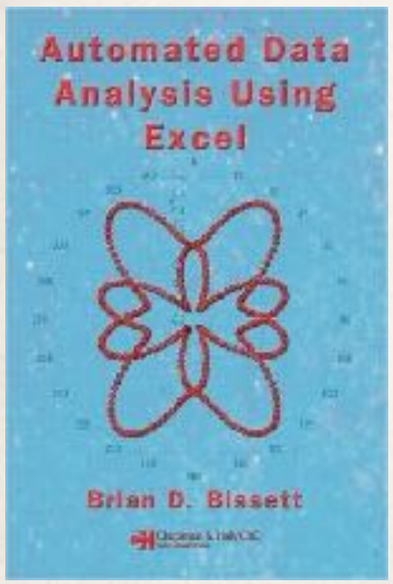



Automated data analysis - data mining.
Can consider large volumes of data with large numbers of variables

# Data analysis? Yes.

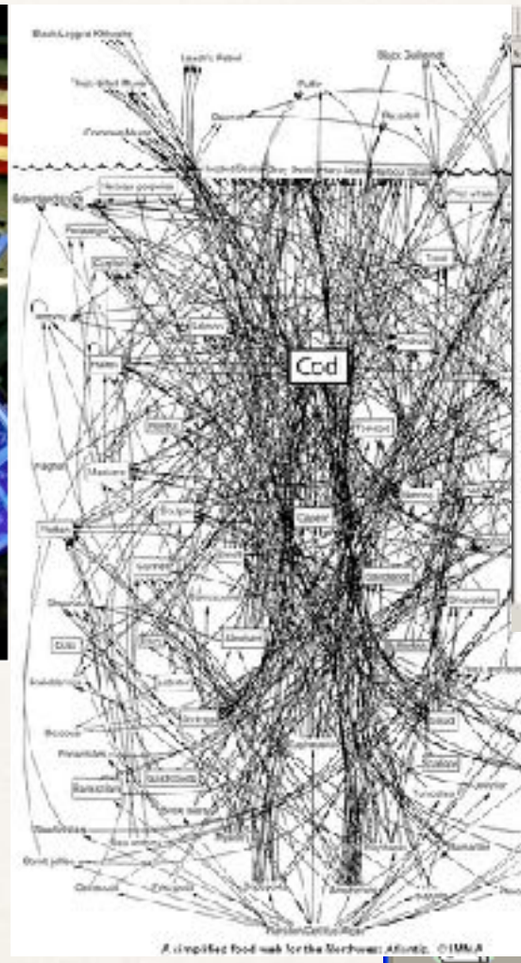
Instinct: Hard-wired data analysis

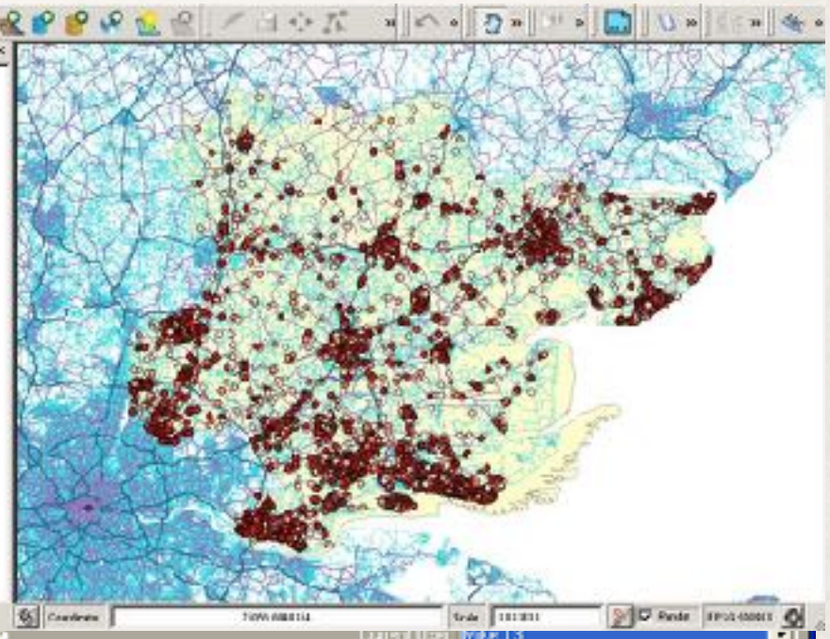
Learning: adaptive data analysis

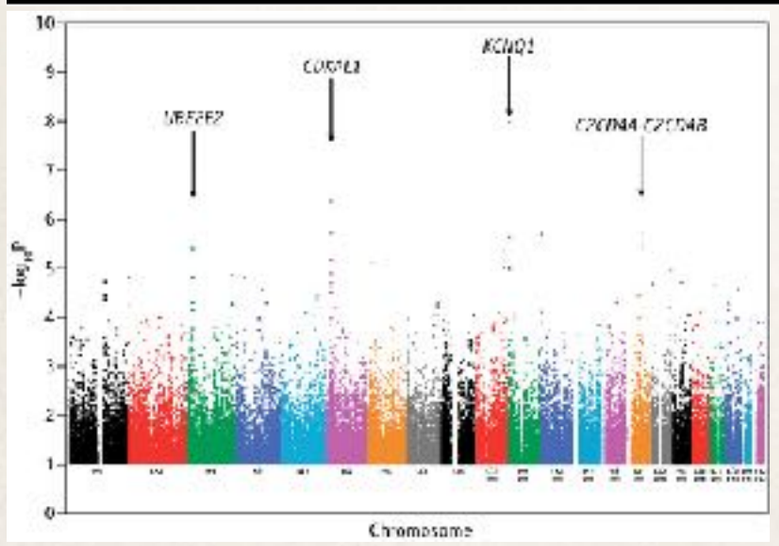


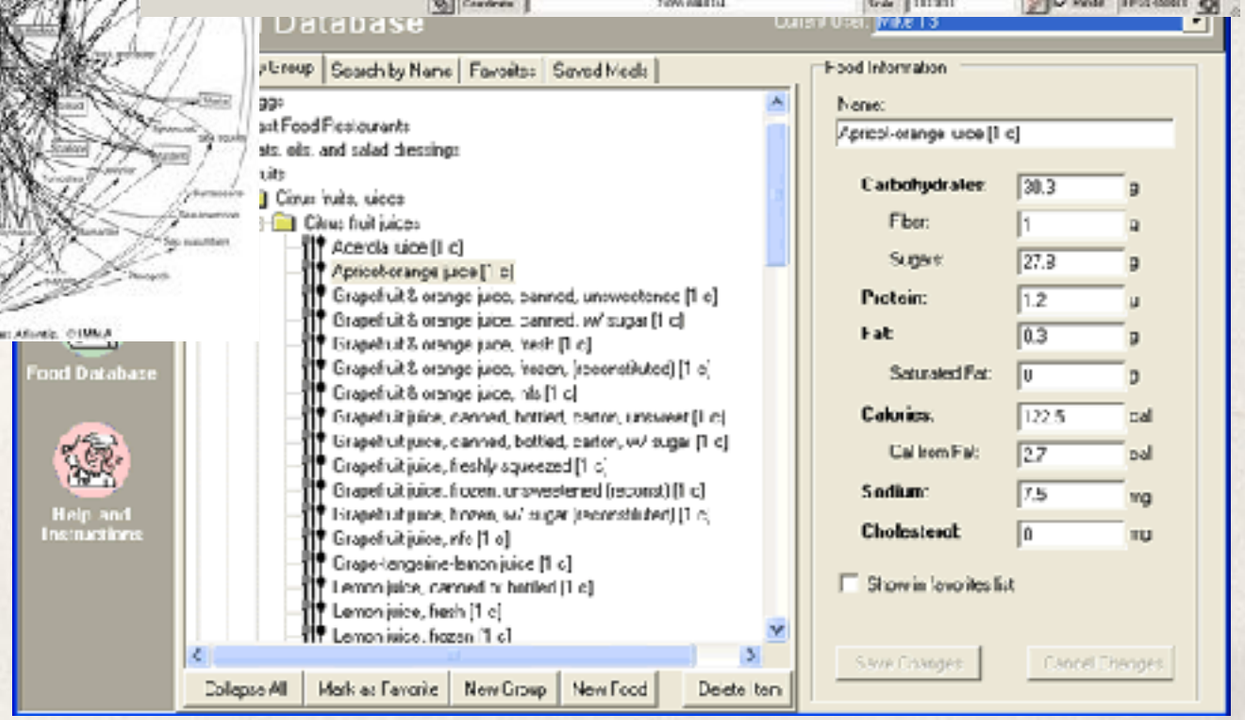

Automated data analysis - data mining.
Can consider large volumes of data with large numbers of variables

# What does all the data from the data revolution represent?







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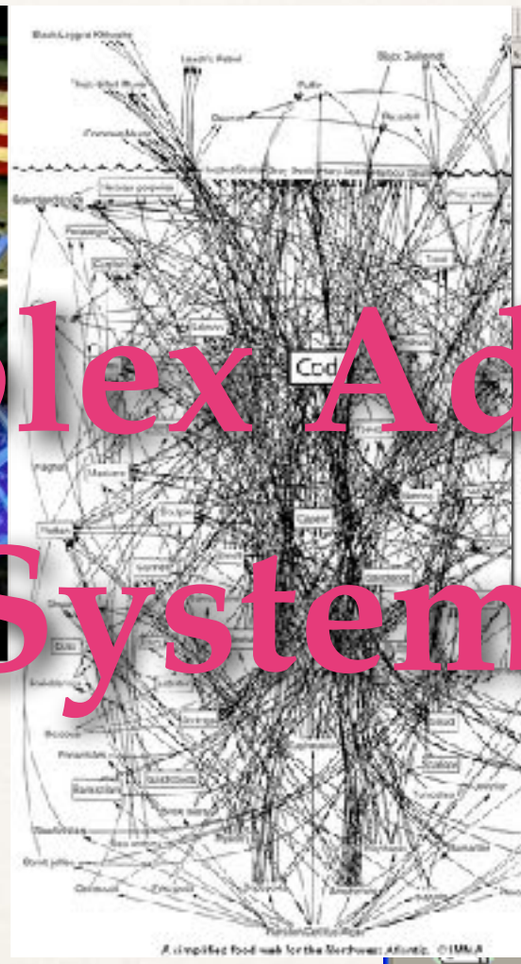
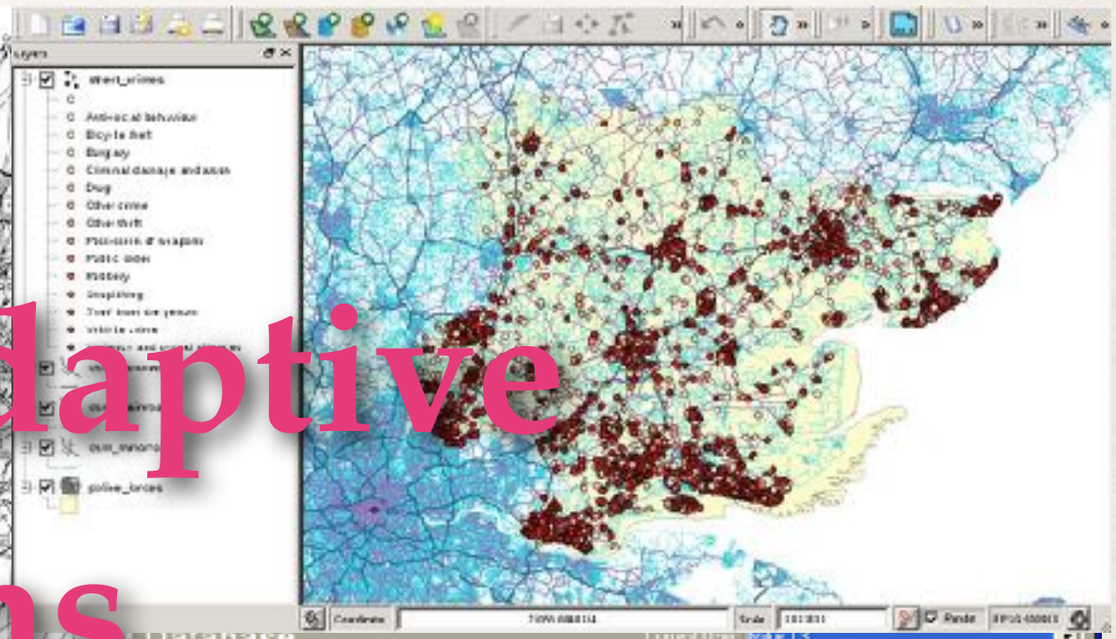
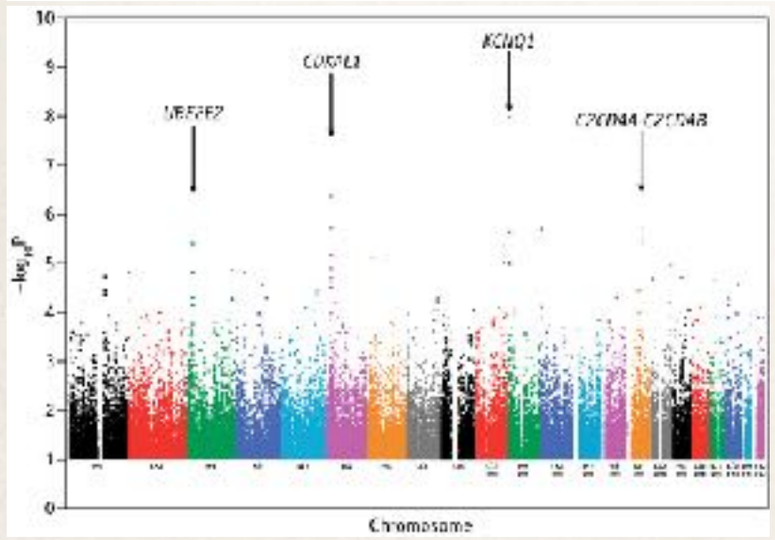
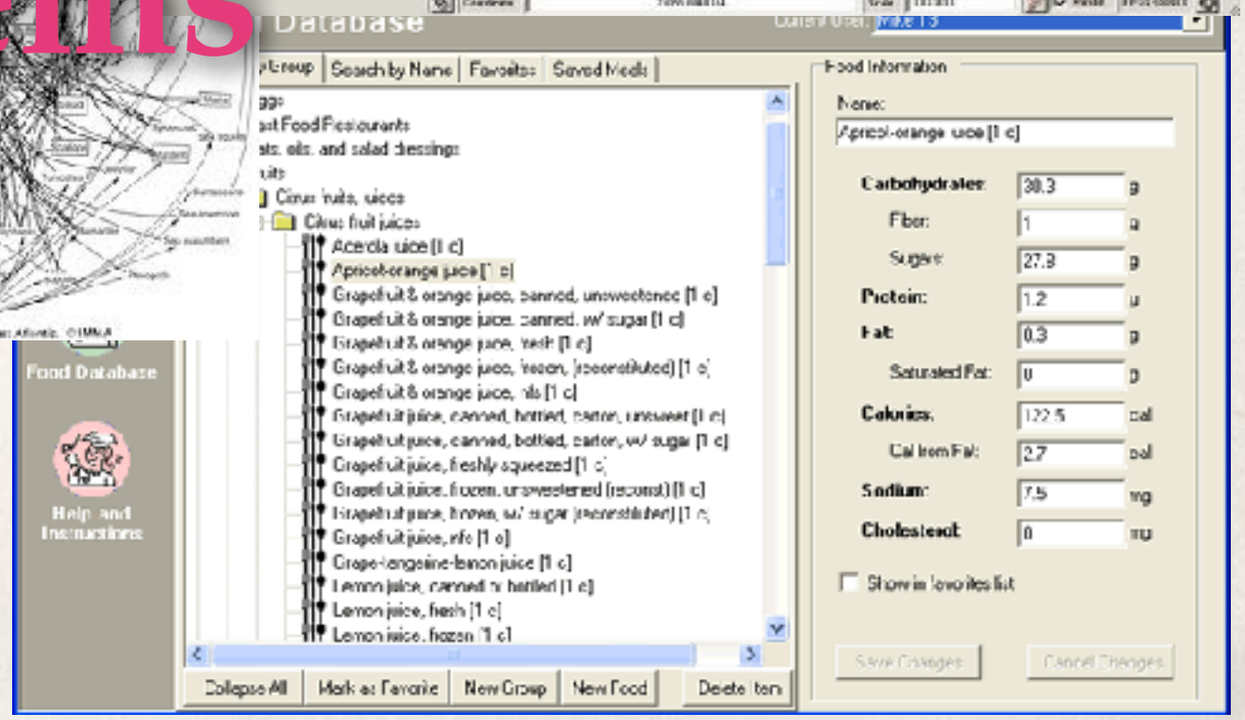


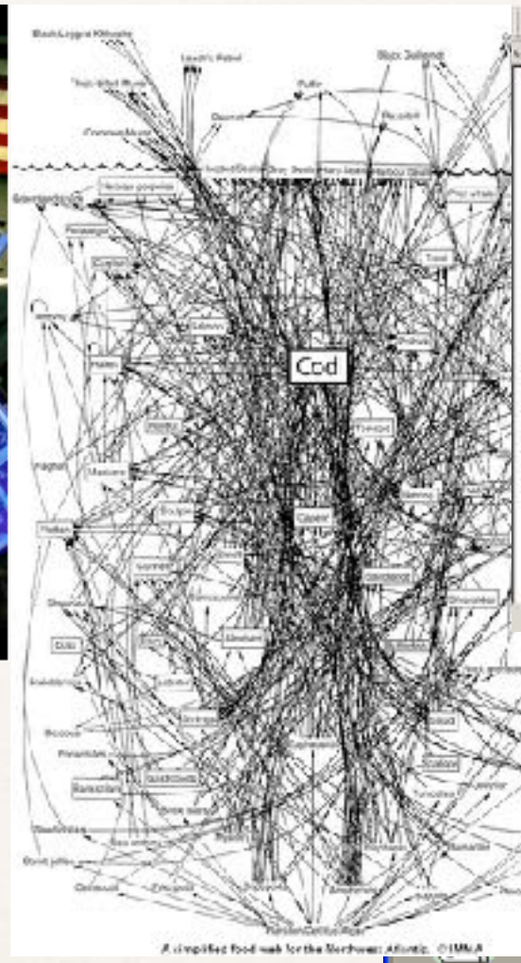


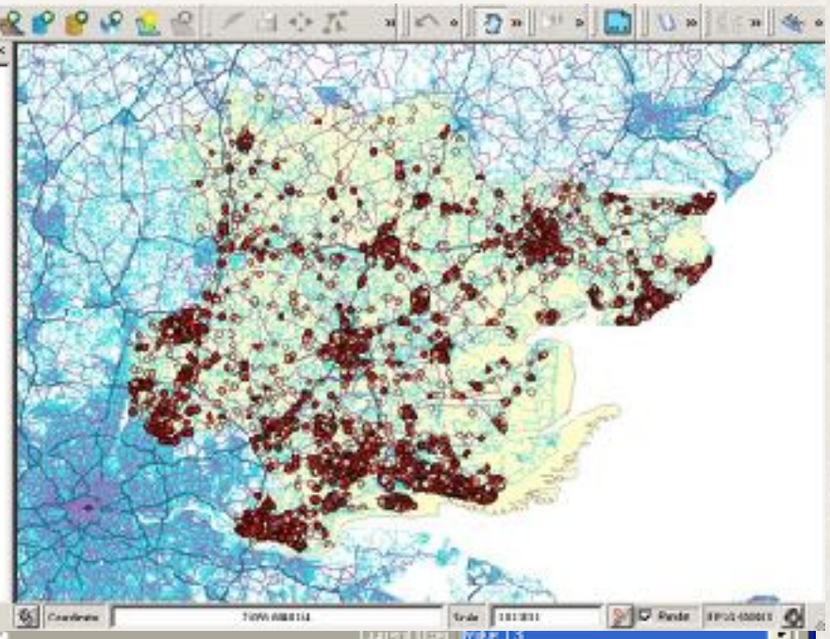


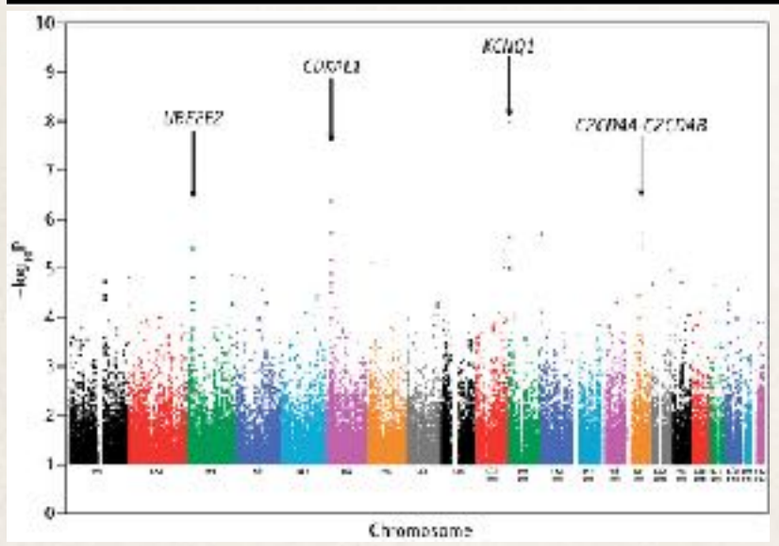



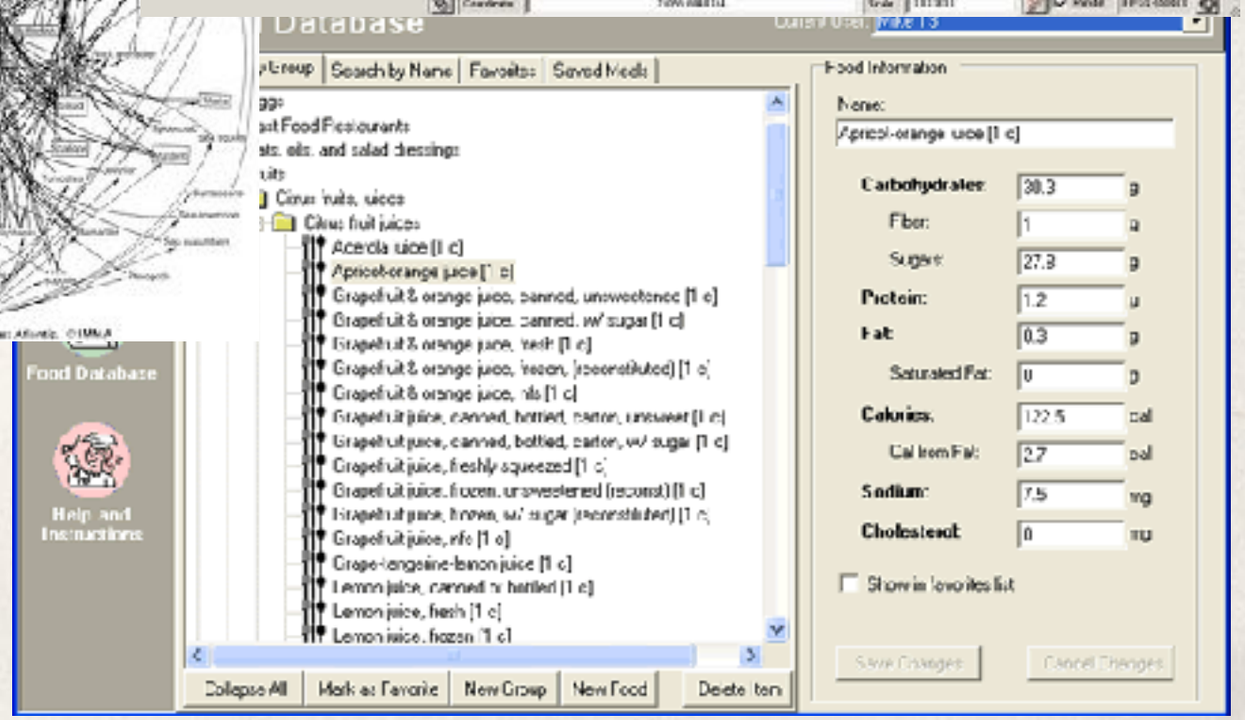

# Complex Adaptive Systems

# What does all the data from the data revolution represent?







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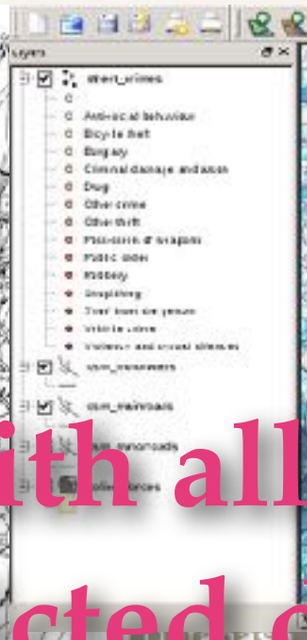
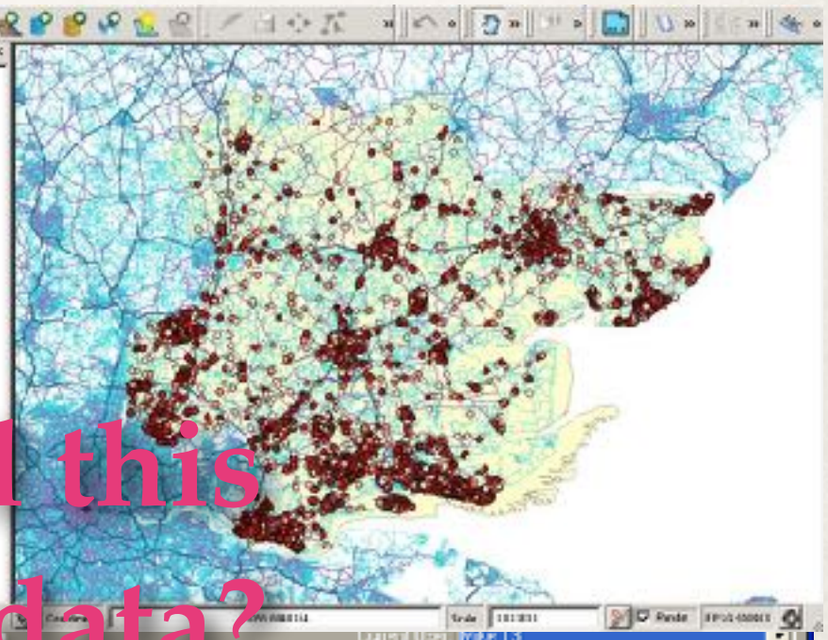
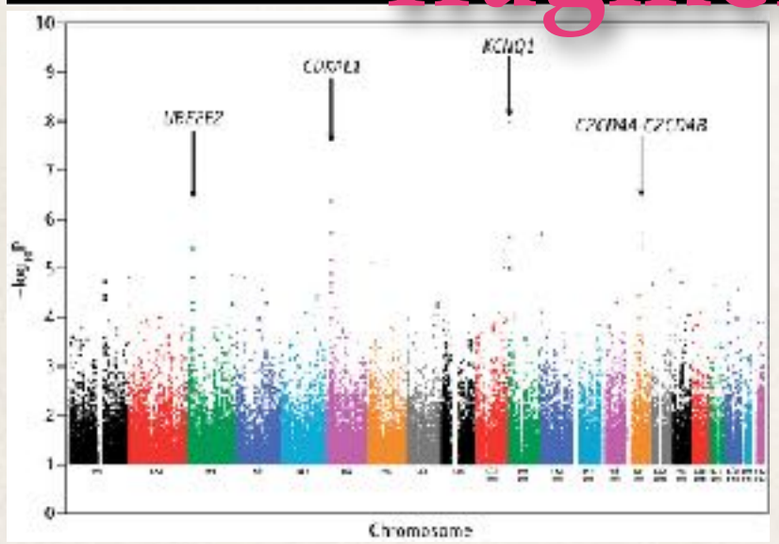
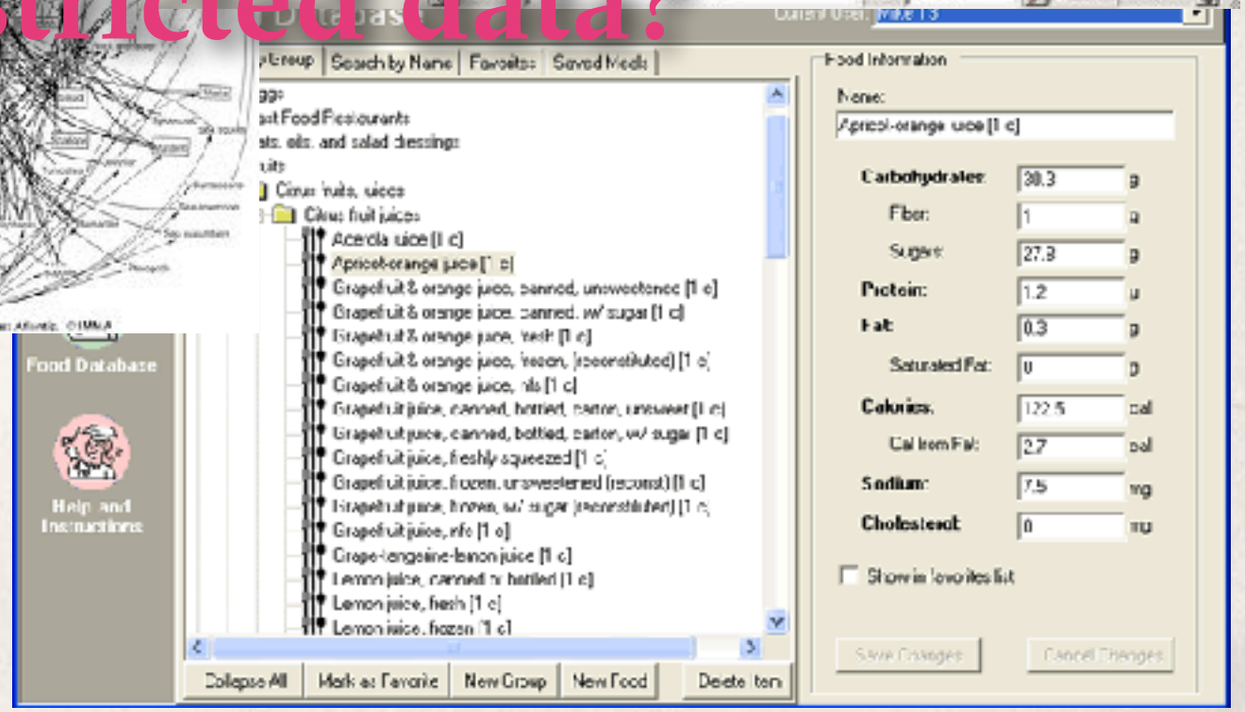


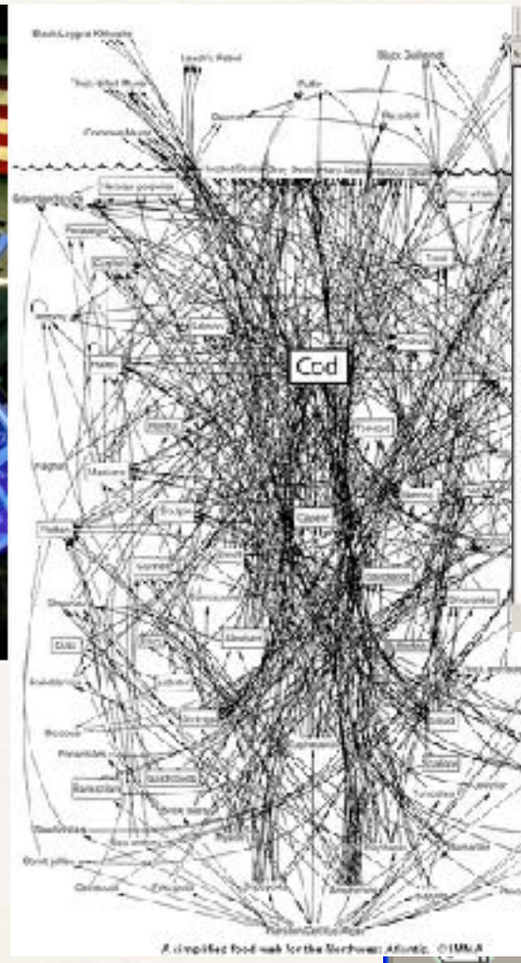


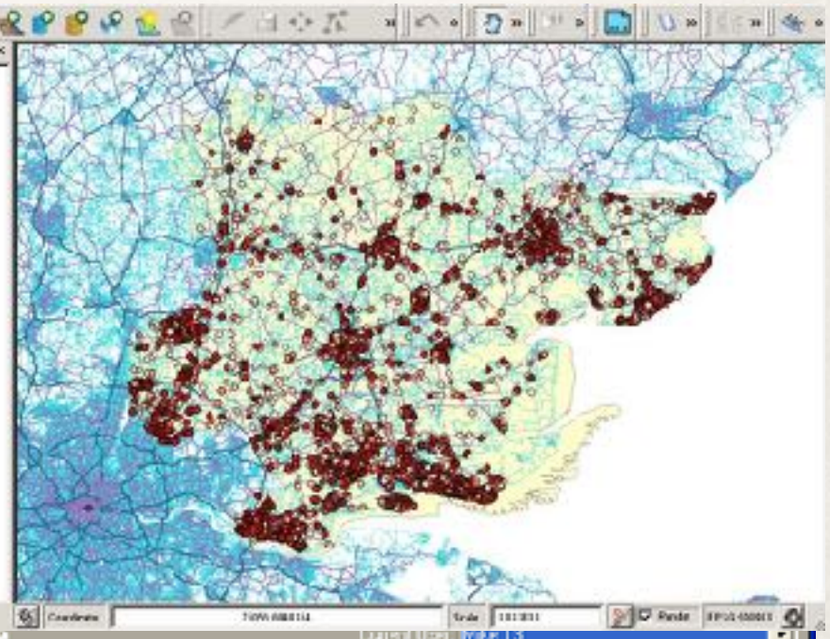


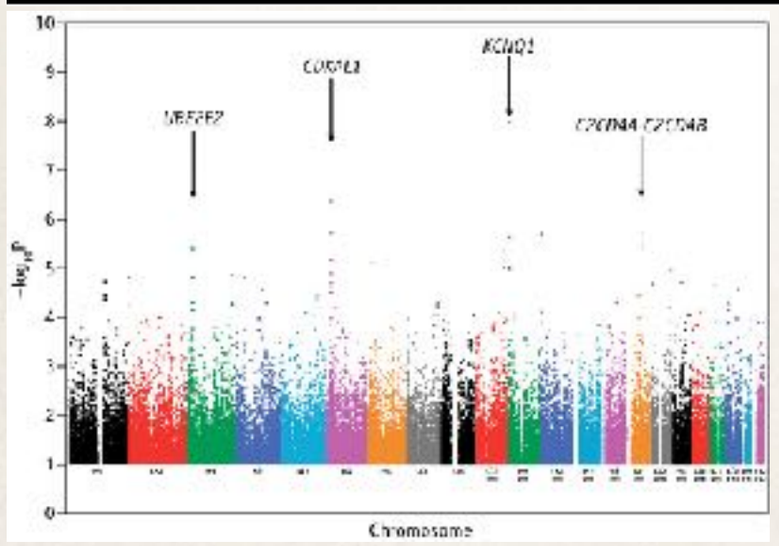



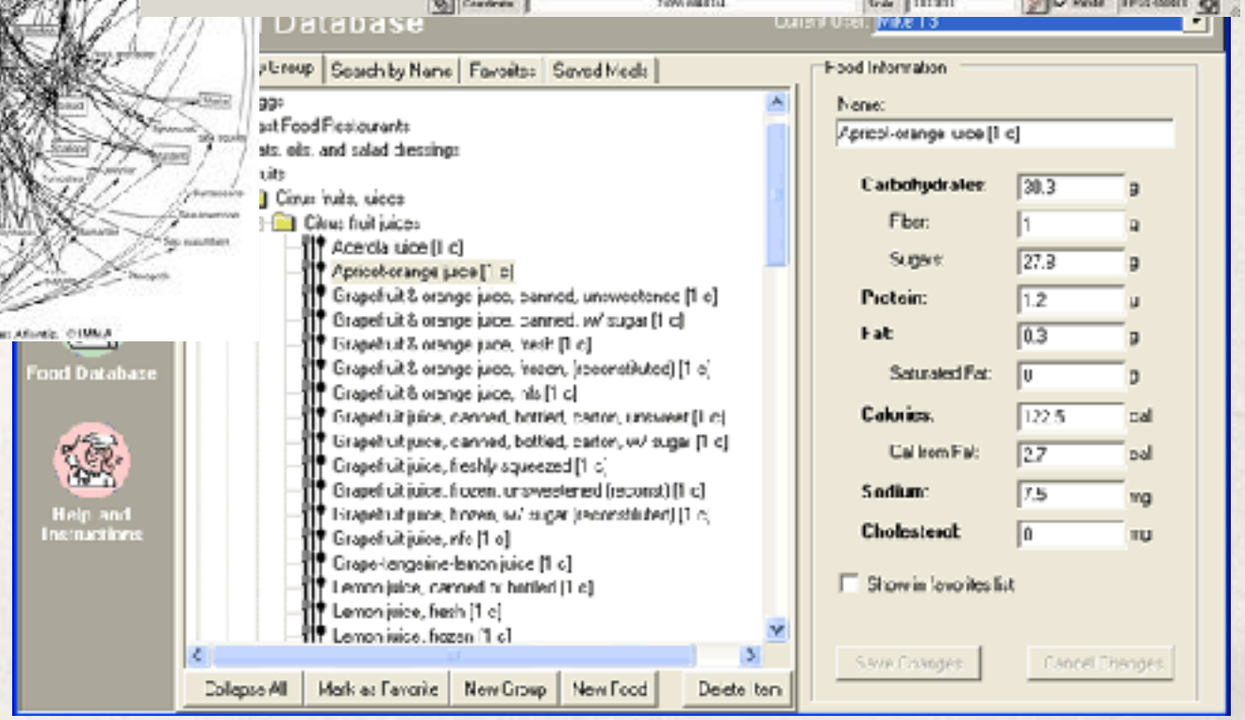

## What do we do with all this fragmented, restricted data?

# What does all the data from the data revolution represent?







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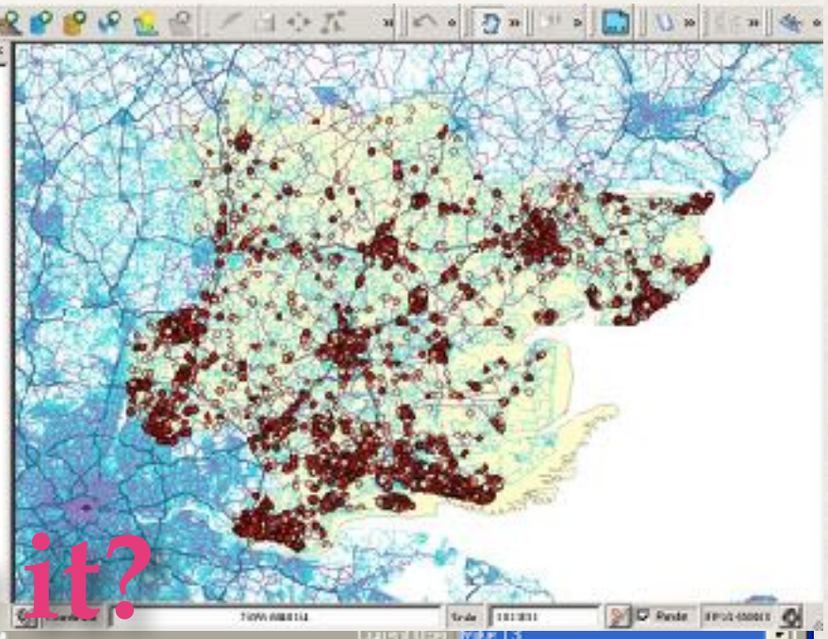
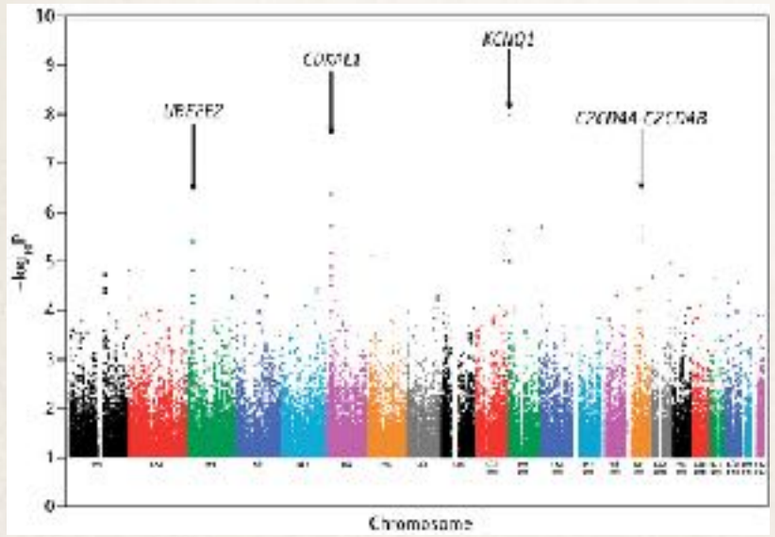
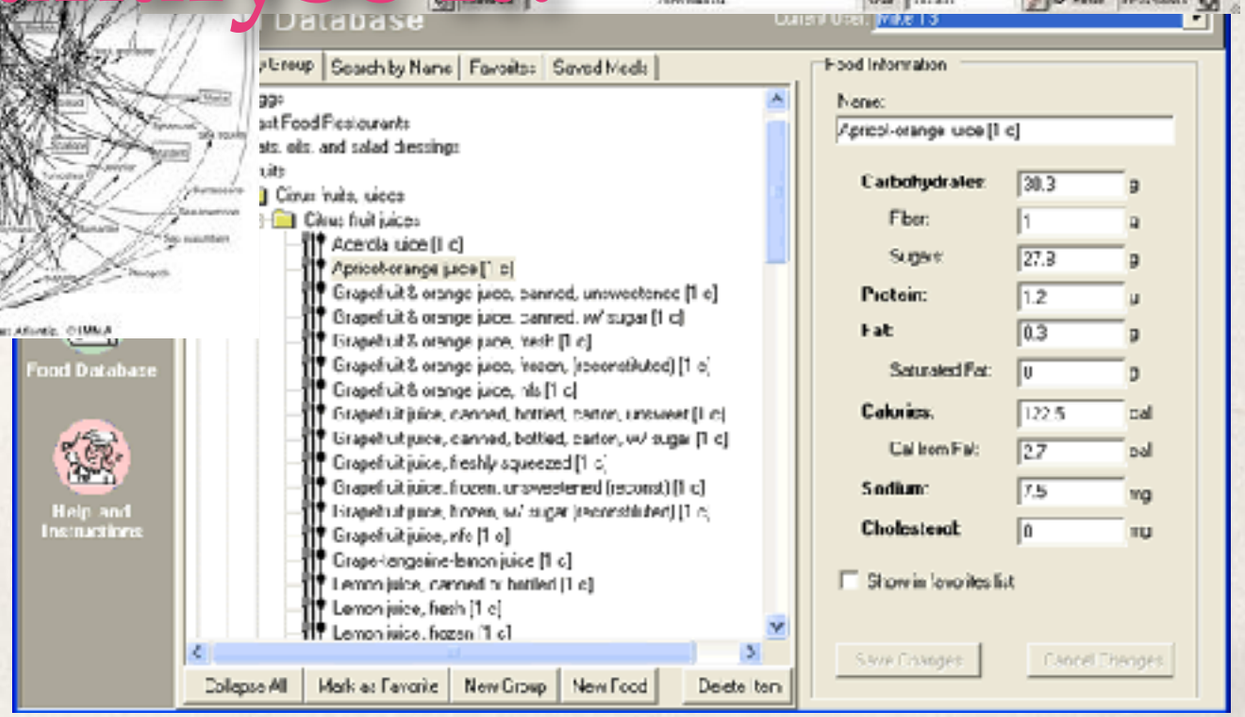


How do we analyse it?



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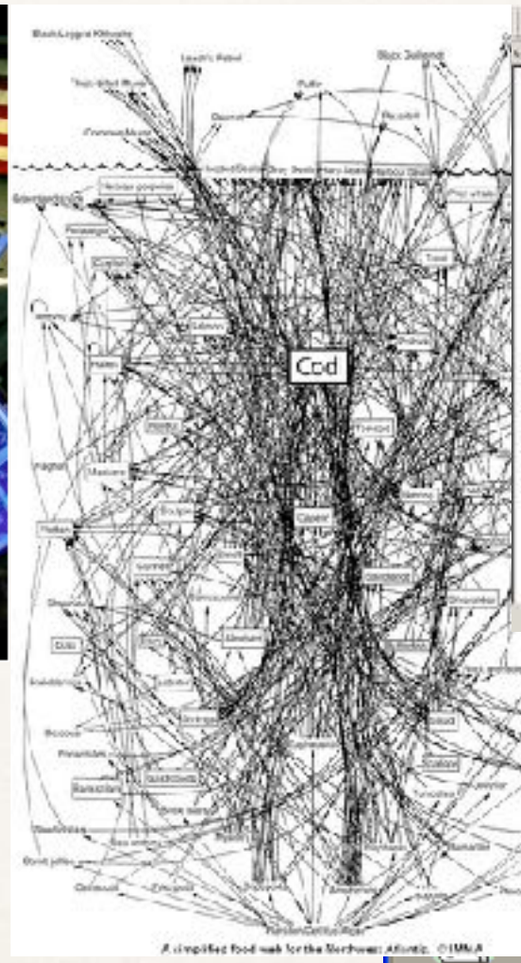
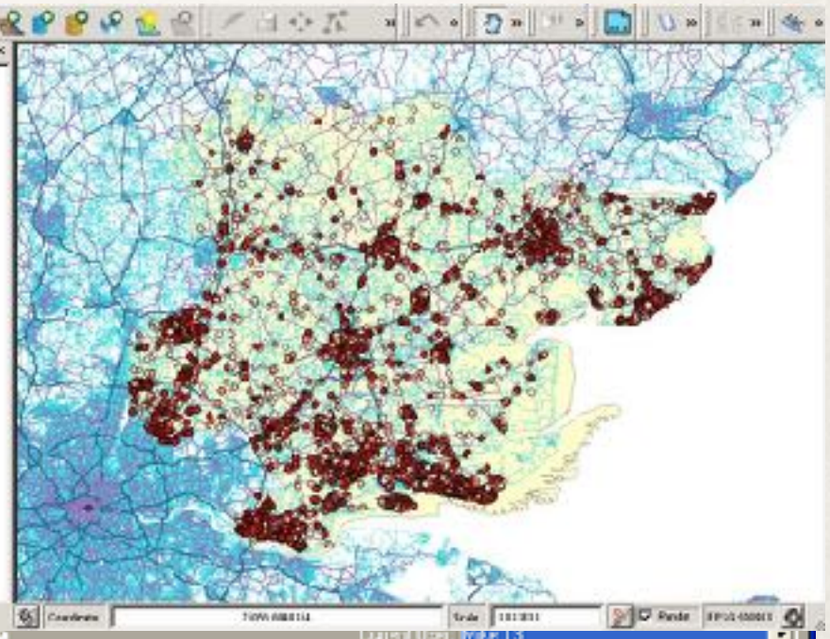
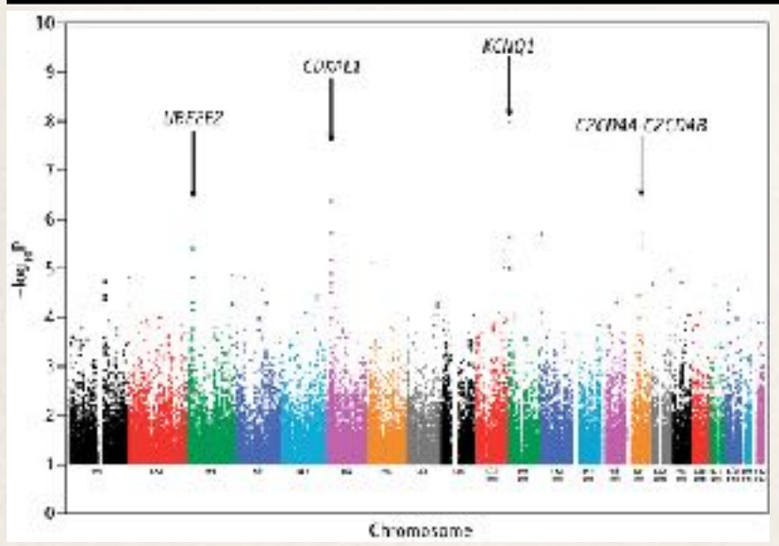
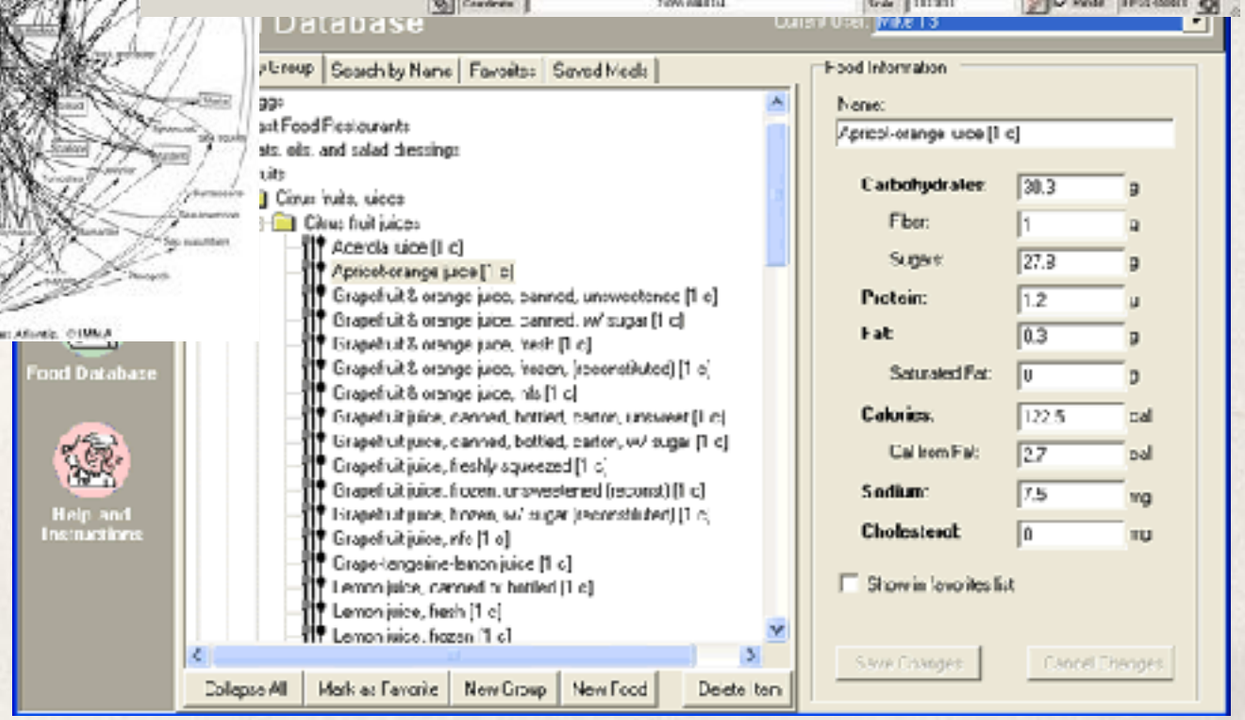






# In Complex Adaptive Systems we need a lot of data because...

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

**There's a lot you can say!**

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

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

Imagine what you can say about a city

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

**Imagine what you can say about a city**

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

**Imagine what you can say about a city**

versus

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

**Imagine what you can say about a city**

versus

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

**Imagine what you can say about a city**

versus

**a crystal as big as a city!**

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

**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  Obesity  Father had diabetes

Angina  Leukaemia  SNP Rs7903146  45 mins exercise per week

## Many effects  Many causes

## 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

# What distinguishes complex from non-complex phenomena?

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?

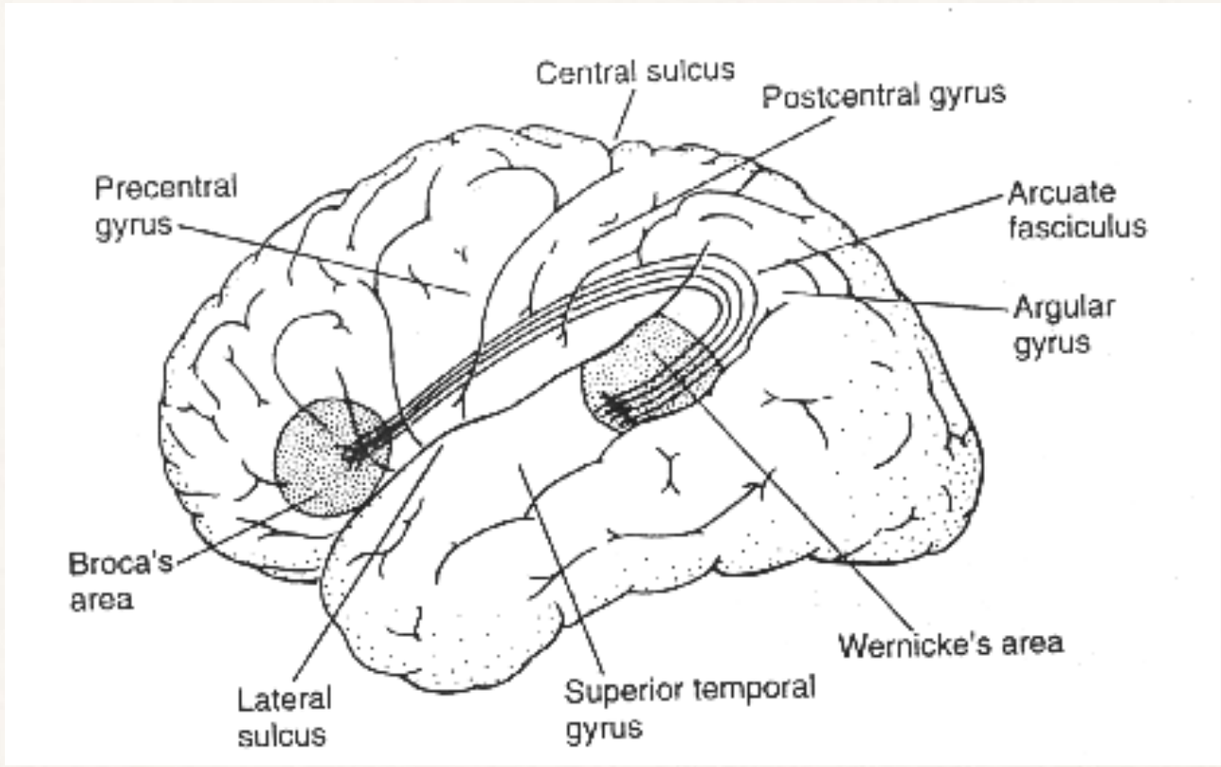
**If it is, then...**

**How do we measure it?**

**What is a good measuring apparatus…?**

# For Symbolic Complexity

**To be or not to be that is the question.**

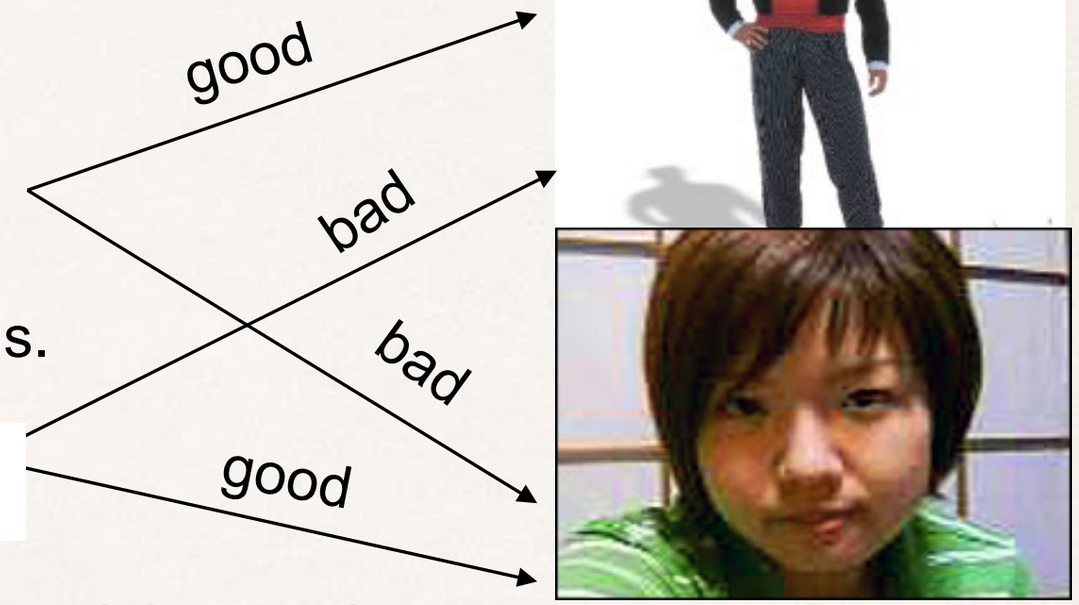



This apparatus is surely capable of measuring complexity. Or maybe not…?

# How good is your apparatus?

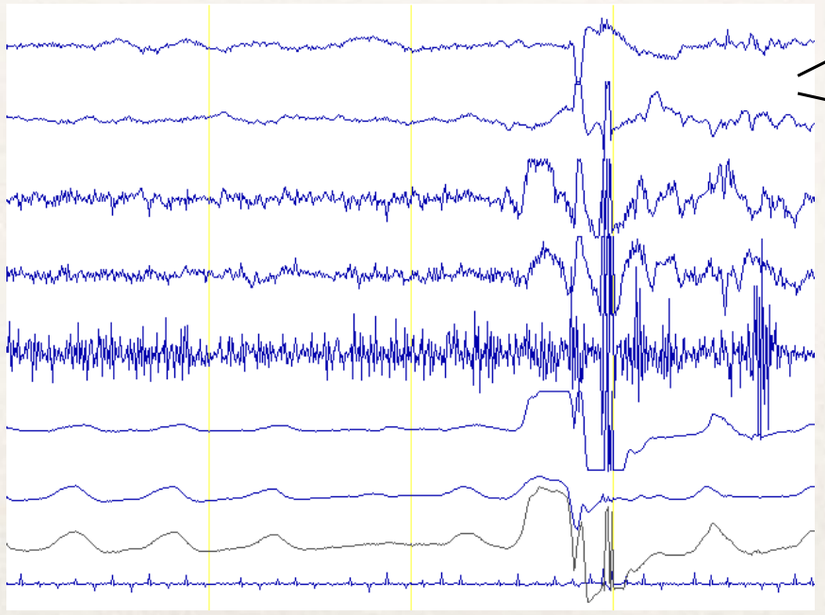
- To be or not to be that is the question.
- Para ser o no ser que es la pregunta.
- Om te zijn of te zijn niet dat de vraag is.

あるためまたはないため質問である




- Because of a certain or because it is not, it is question.
- Because or it is not for the sake of, that having asked and being convinced.
- 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.

# Is this different to physics?

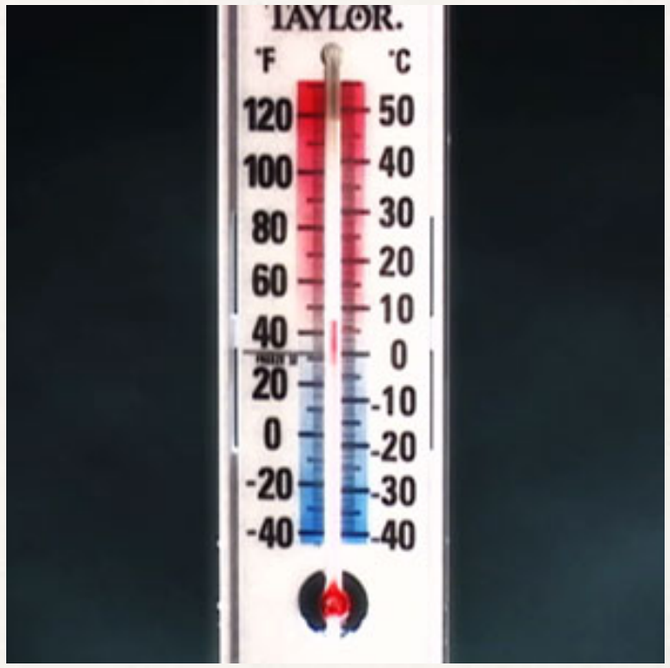


good

bad

bad

good



# Modeling complexity

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

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

# we need a space of states

# 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?

$$\mathbf{d}_i(t+\Delta t) = \sum_{j \neq i} \frac{\mathbf{c}_j(t) - \mathbf{c}_i(t)}{|(\mathbf{c}_j(t) - \mathbf{c}_i(t))|} + \sum_{j=1} \frac{\mathbf{v}_j(t)}{|\mathbf{v}_j(t)|}$$

Competition between an effective repulsion and attraction between "particles"

$$\hat{\mathbf{d}}_i(t+\Delta t) = \mathbf{d}_i(t+\Delta t)/|\mathbf{d}_i(t+\Delta t)|$$

$c_i(t)$, $v_i(t)$ – 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

# Predictability in physical systems versus Complex Adaptive Systems

## The difference between complex and simple systems is the difference between "being" and "doing"

# Predictability in physical systems versus Complex Adaptive Systems

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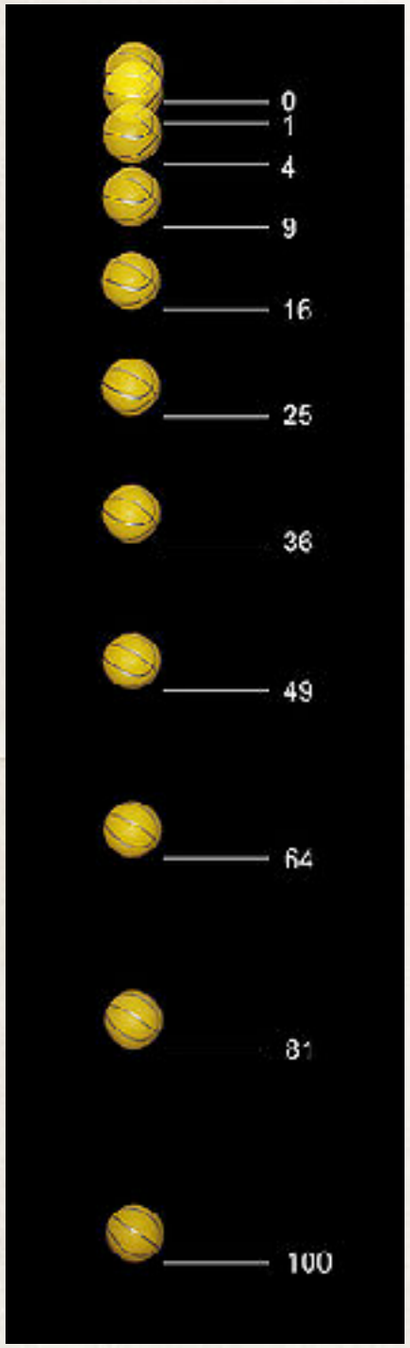
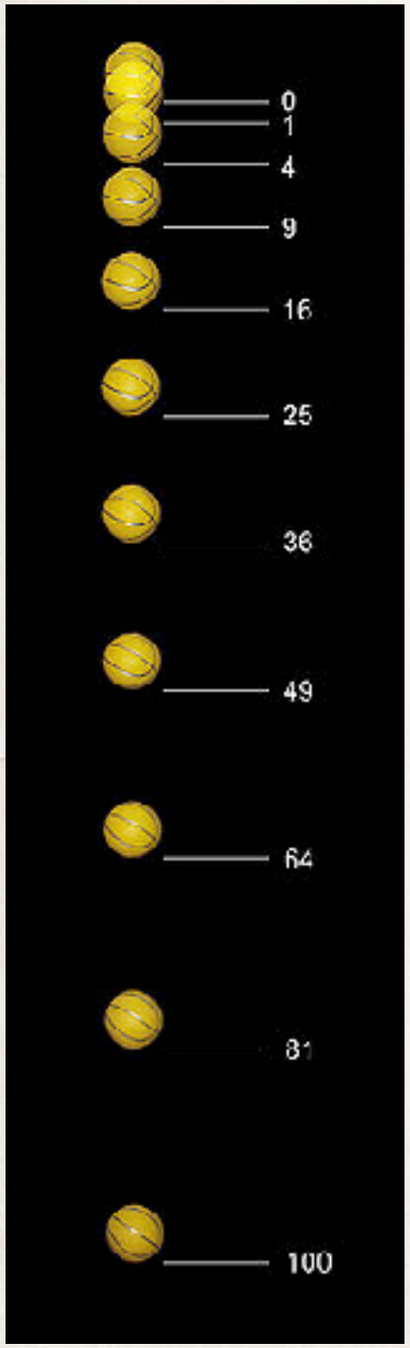
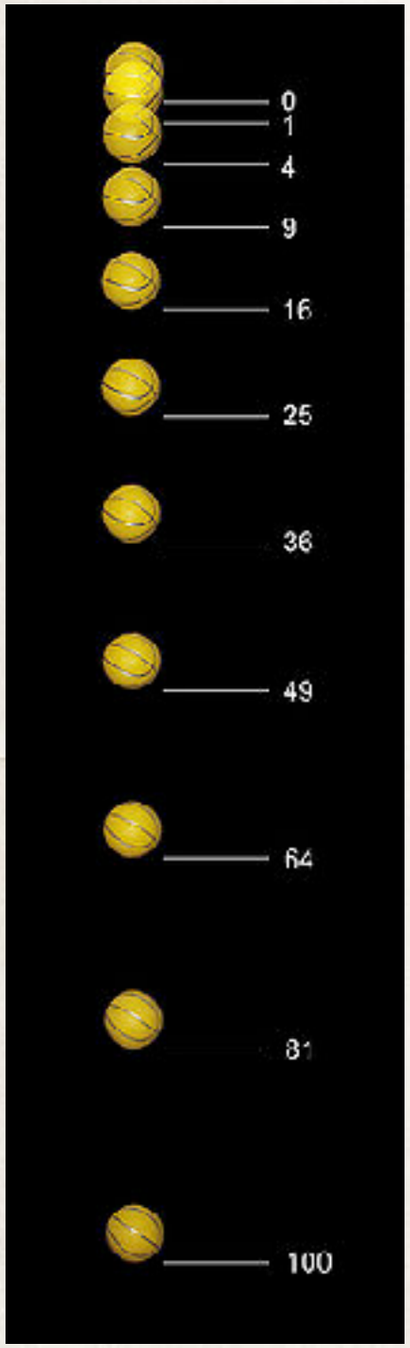


# Predictability in physical systems versus Complex Adaptive Systems




## Mechanistic

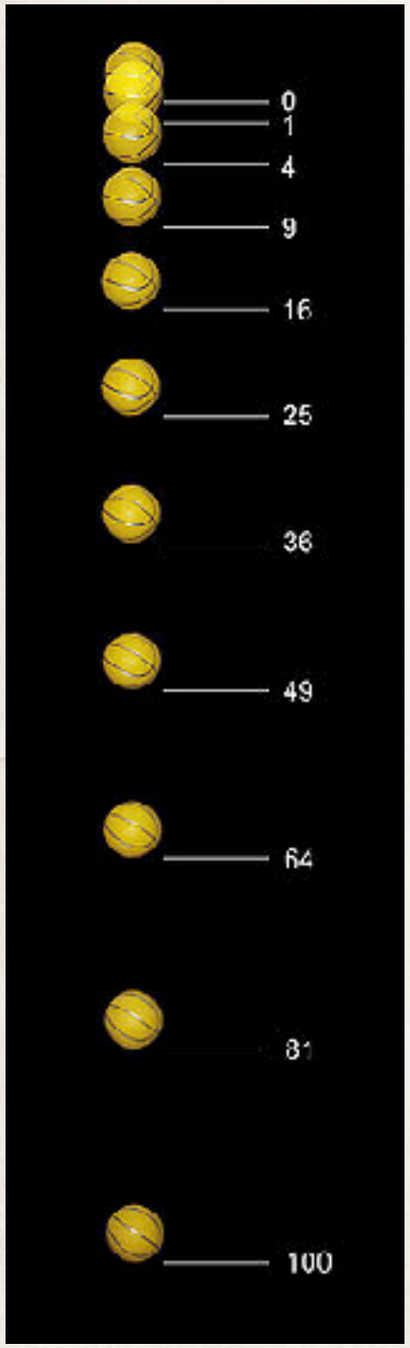
# Predictability in physical systems versus Complex Adaptive Systems




**Mechanistic**

**Adaptive**

# Predictability in physical systems versus Complex Adaptive Systems

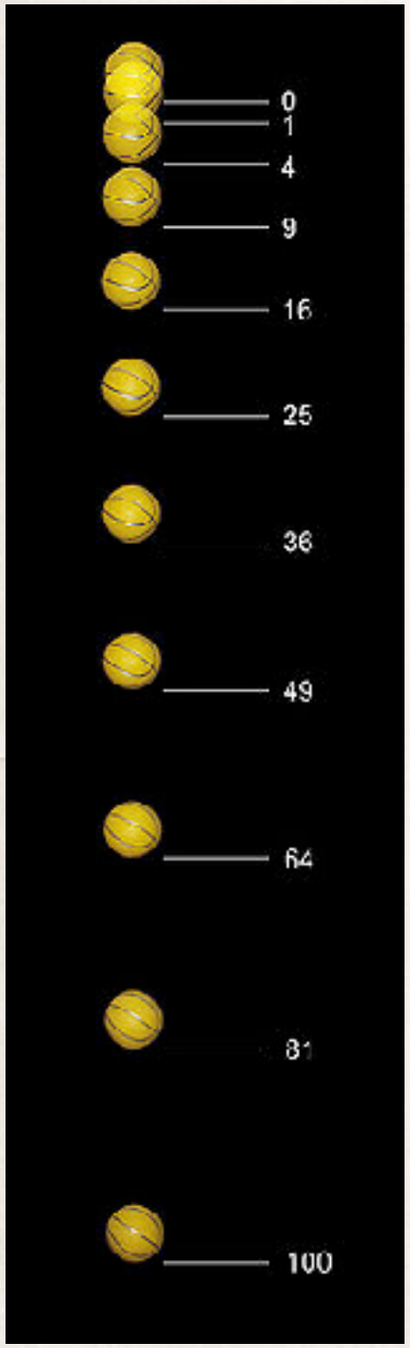



**Mechanistic**

**Adaptive**

## The cat obeys the same laws of physics as the ball

# Predictability in physical systems versus Complex Adaptive Systems




**Mechanistic**

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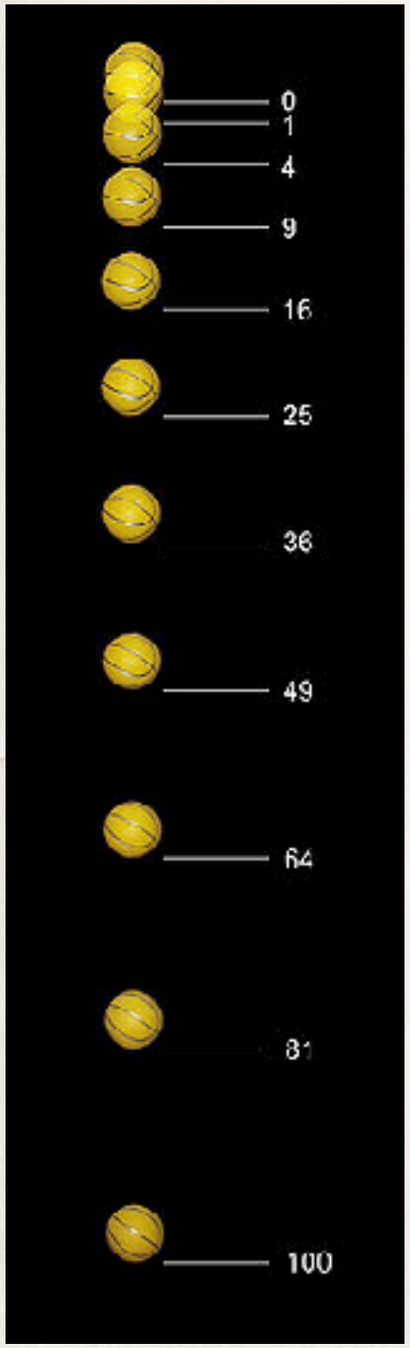
# Predictability in physical systems versus Complex Adaptive Systems

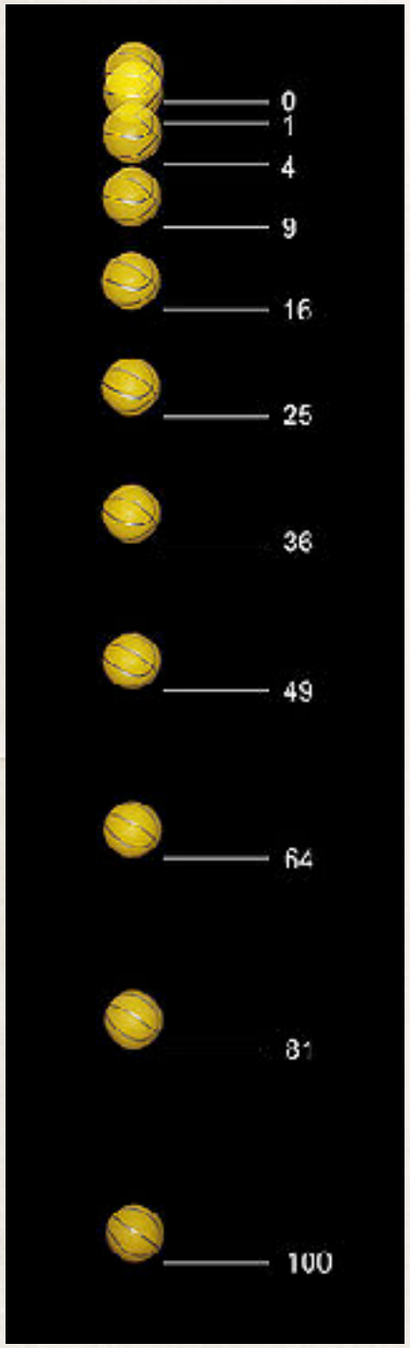



**Mechanistic**

**Adaptive**

## But its not a “slave” to them

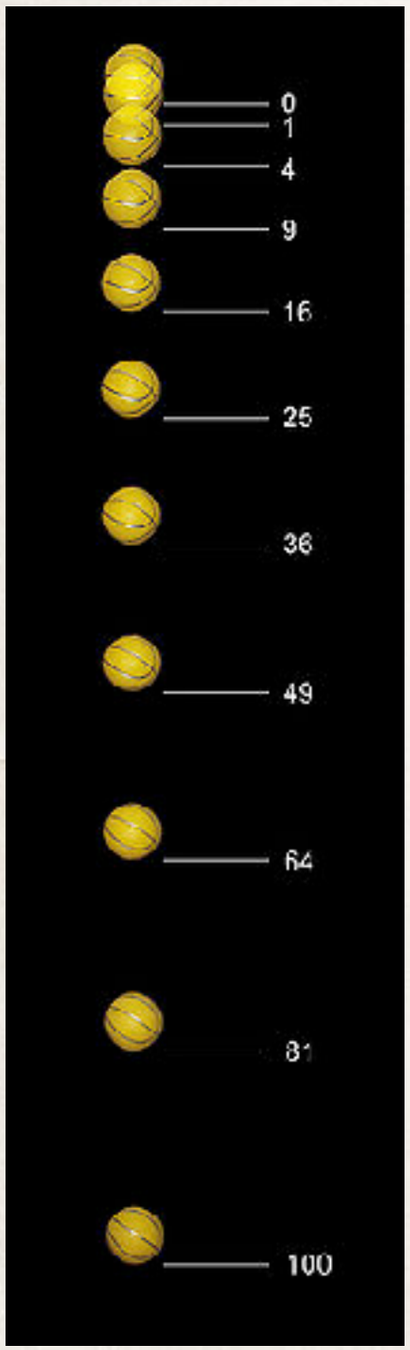
# Predictability in physical systems versus Complex Adaptive Systems




**Mechanistic**

**Adaptive**

# Predictability in physical systems versus Complex Adaptive Systems




Mechanistic

Adaptive

## The *evolution* of function is the revolution that allowed systems to escape the tyrrany of the laws of physics. Complexity is a consequence of that revolution.

# The Difference Between "Being" and "Doing"

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

# Evolved Virtual Creatures

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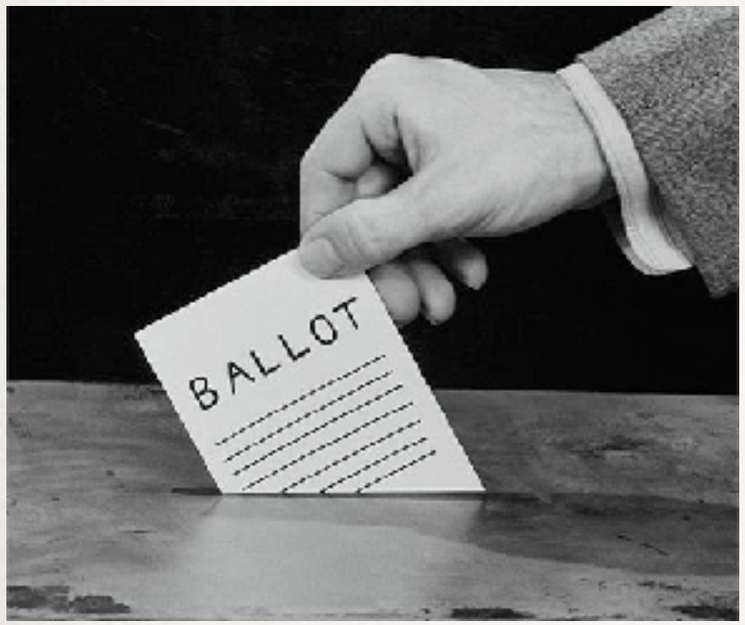
# Complex Adaptive Systems...
# make "decisions"

# Complex Adaptive Systems...
# make "decisions" both at the individual and collective levels

**both at the individual and collective levels**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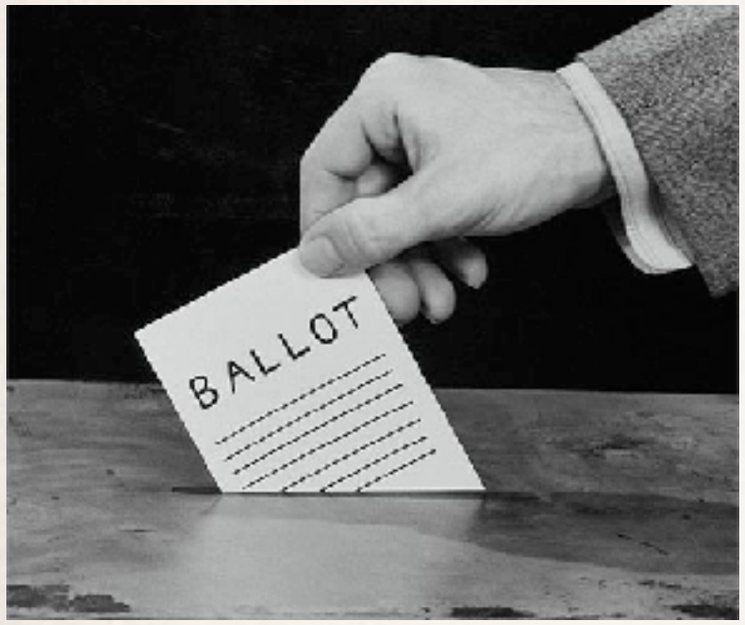
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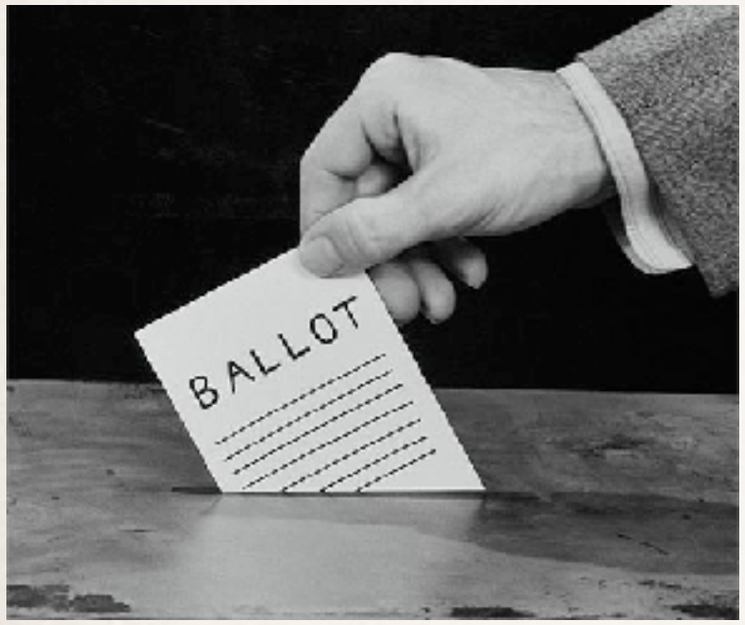
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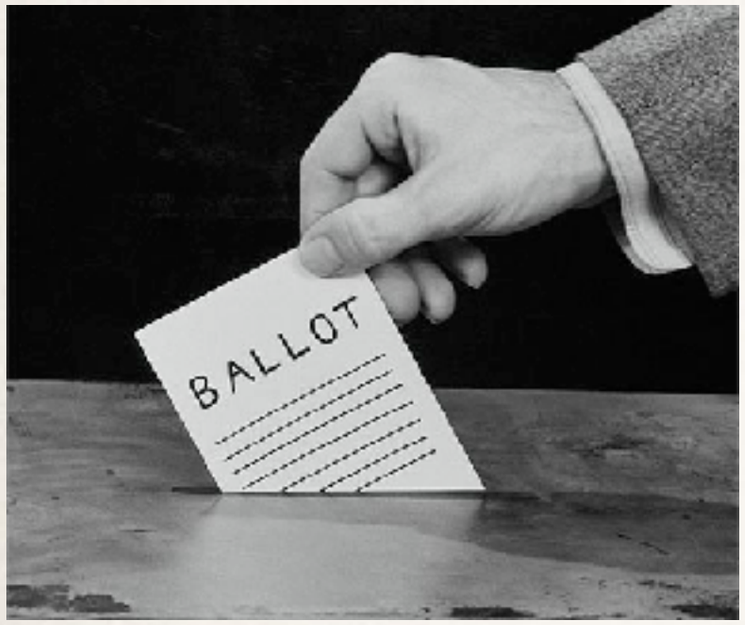
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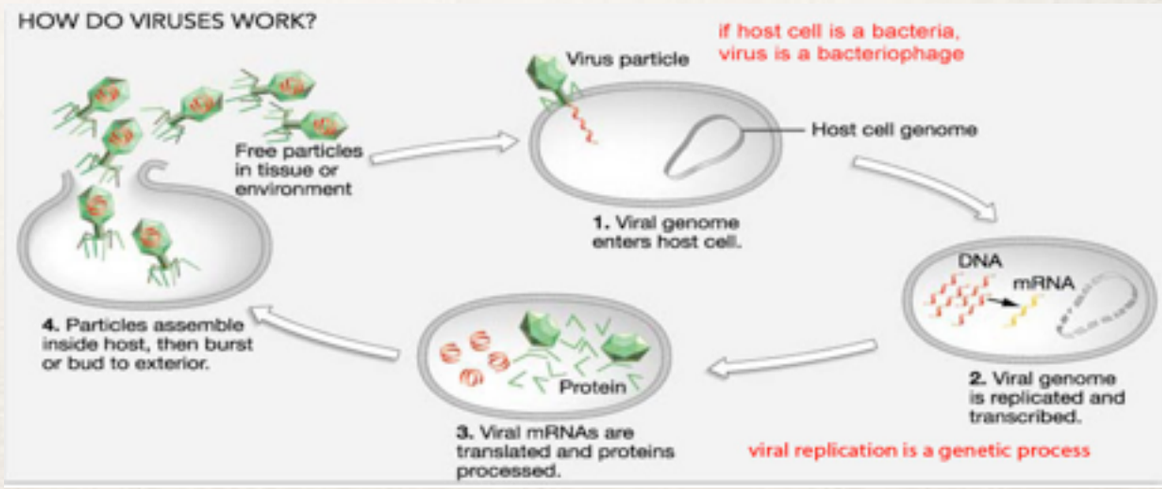
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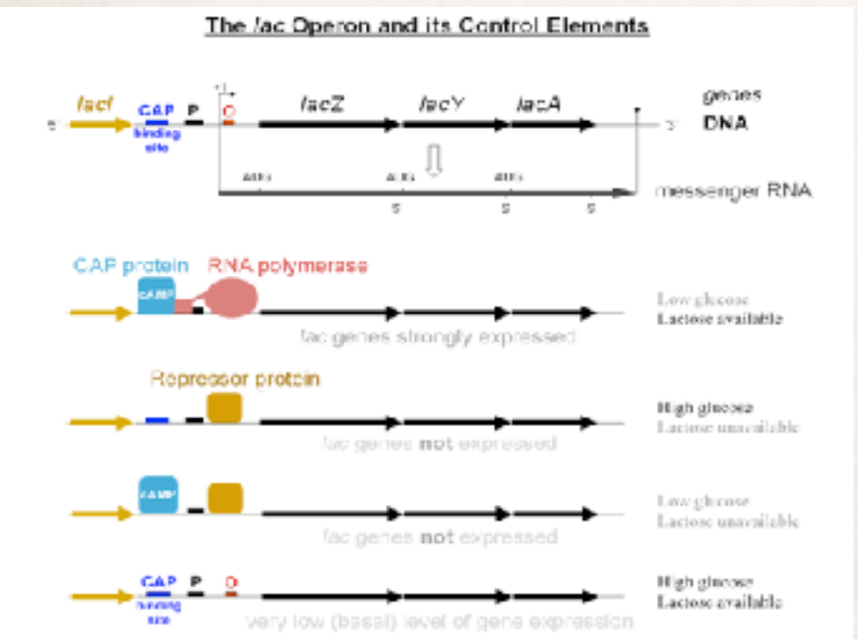
Virus particle
Host cell genome
Free particles in tissue or environment
1. Viral genome enters host cell.
DNA
mRNA
2. Viral genome is replicated and transcribed.
Protein
3. Viral mRNAs are translated and proteins processed.
4. Particles assemble inside host, then burst or bud to exterior.
viral replication is a genetic process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Low glucose
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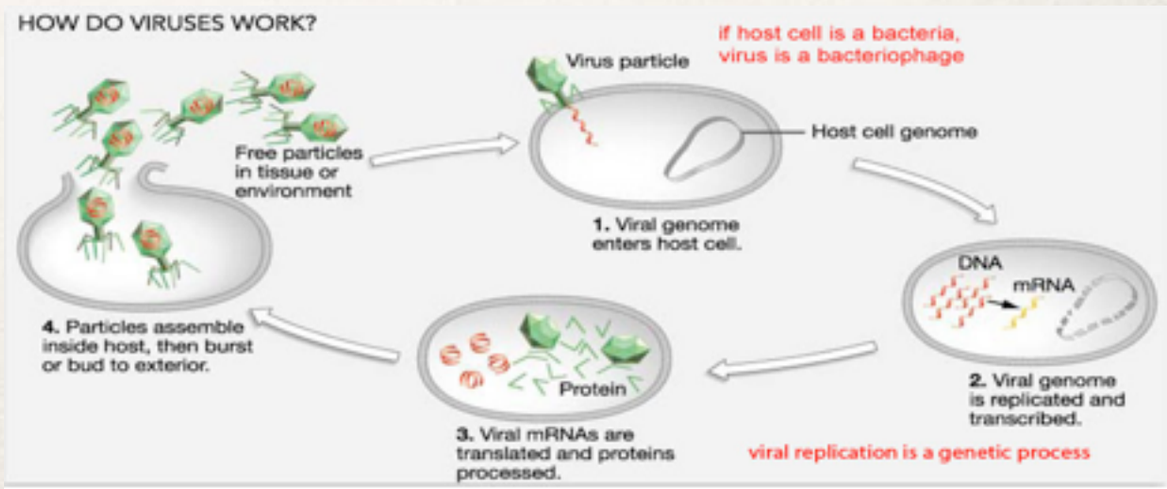
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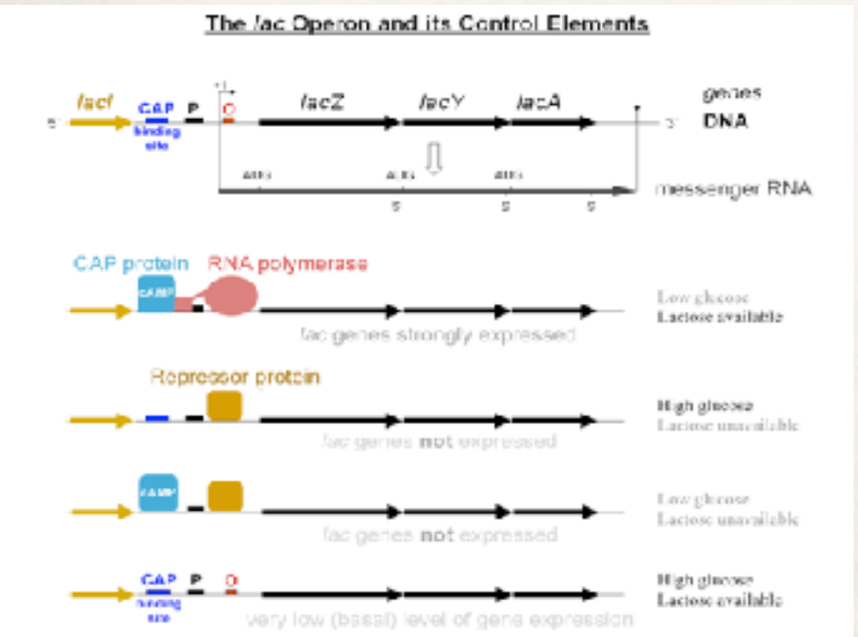
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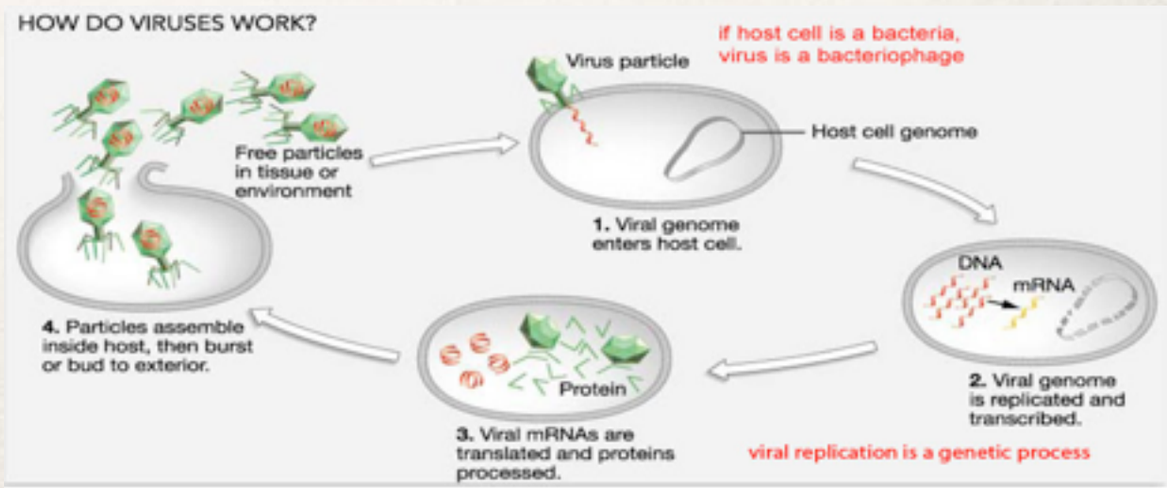
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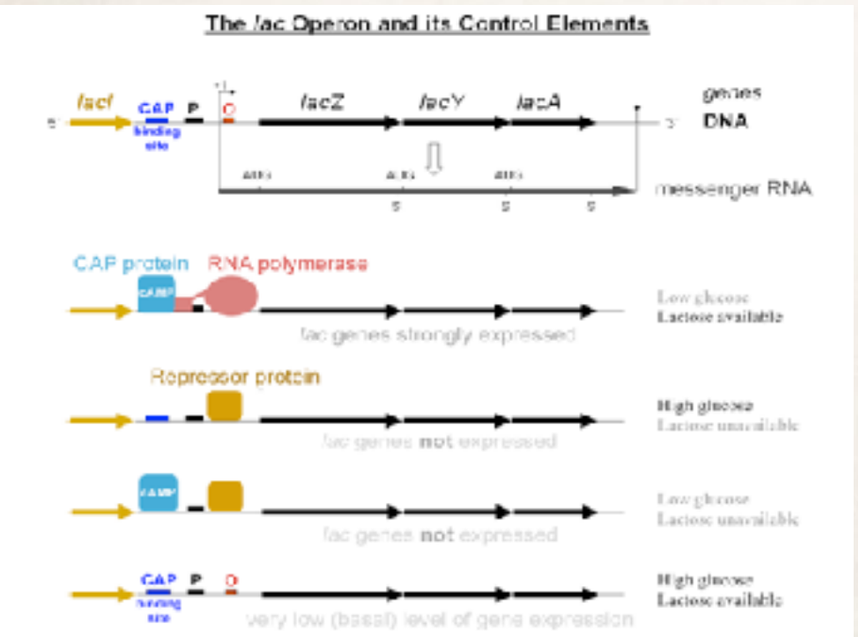
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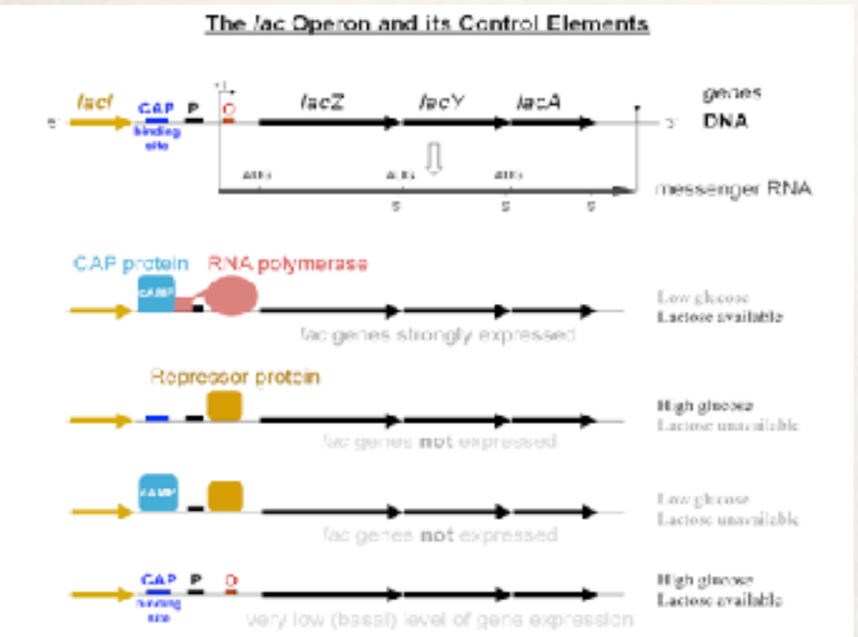
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There are good decisions
and there are bad decisions

# Predictibilidad en los Sistemas Simples versus los Sistemas Complejos

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

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Fenomenología: experiencia cotidiana Las leyes de Newton

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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?

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Coca cola

# ¿Qué es predecible?
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Coca cola

Pepsi

# ¿Qué es predecible?
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Coca cola 70% Pepsi

# ¿Qué es predecible?
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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%

# ¿Qué es predecible?
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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?

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Si regresas

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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

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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?

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# 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

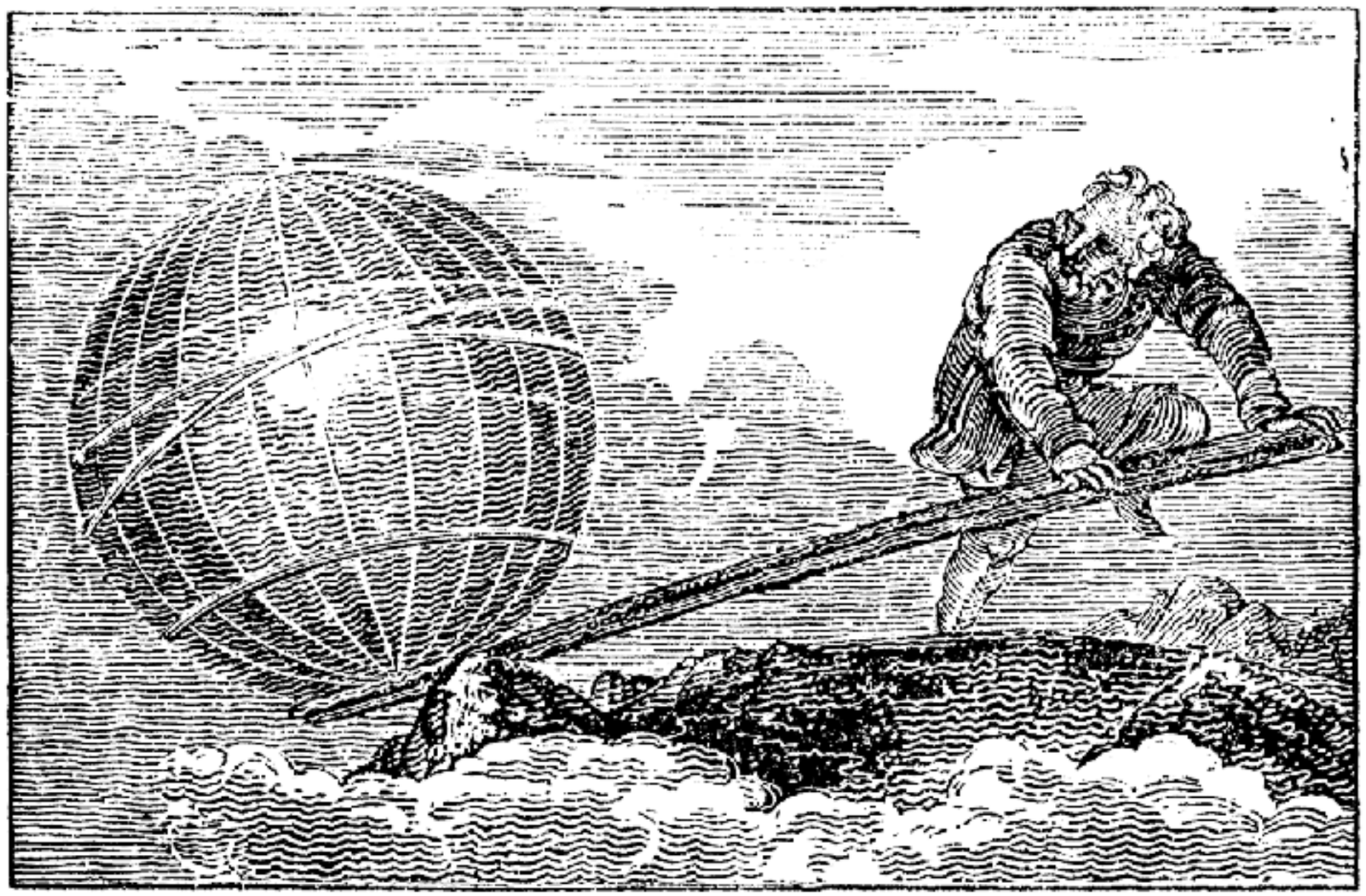
- Complex Adaptive Systems are phenomenologically deep and need a lot of data to describe them…

# 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

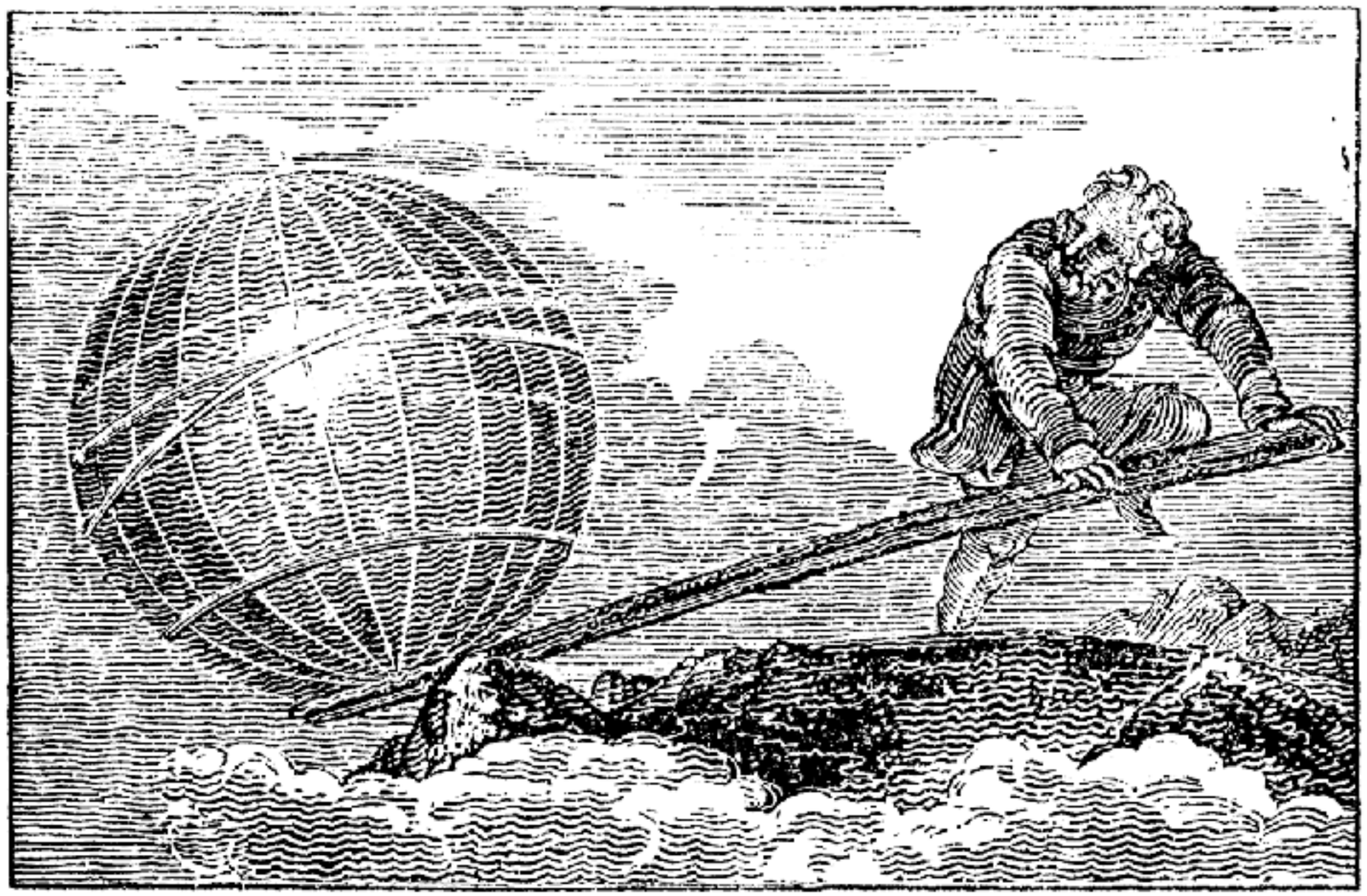
# Conclusions: Complex Adaptive Systems

- 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



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# Give me enough data and I´ll predict anything