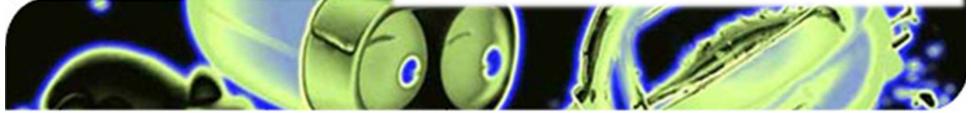


Visualization and interpretability in practical applications

#### WSOM+ 2017

12th International Workshop on Self-Organizing Maps and Learning Vector Quantization, Clustering and Data Visualization (28-30 June 2017)



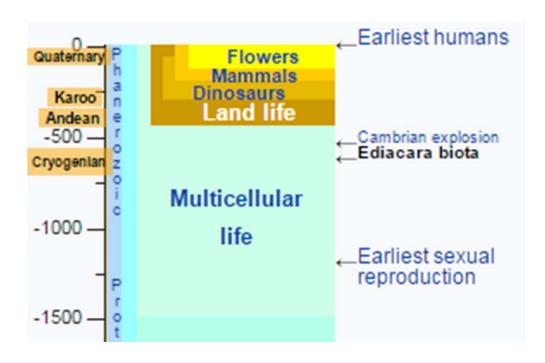


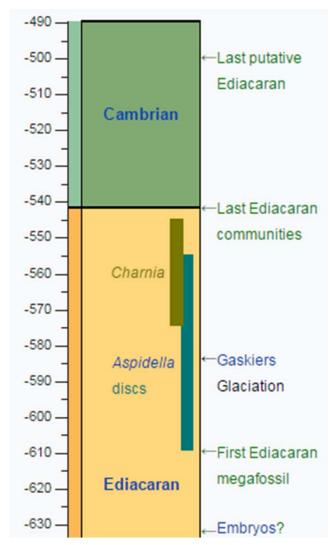




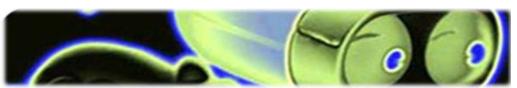


# Context as (pre)history Enter the *ediacaran*









# Context as (pre)history Enter the *ediacaran*Meet *Kimberella*



**Bilaterian**: beyond jellyfish-like radial structures. Bilateral structure as a driver towards more complex nervous systems.

**Early eyes?**: some early evidence of photoreceptors associated to nervous systems. Still unresolved: did the visual system developed independently from the neuromotor control system?

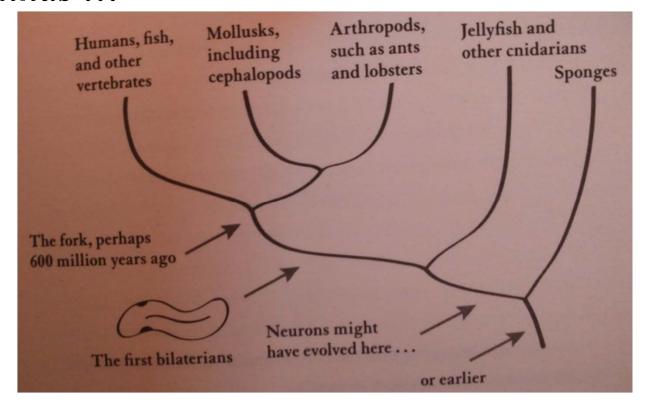


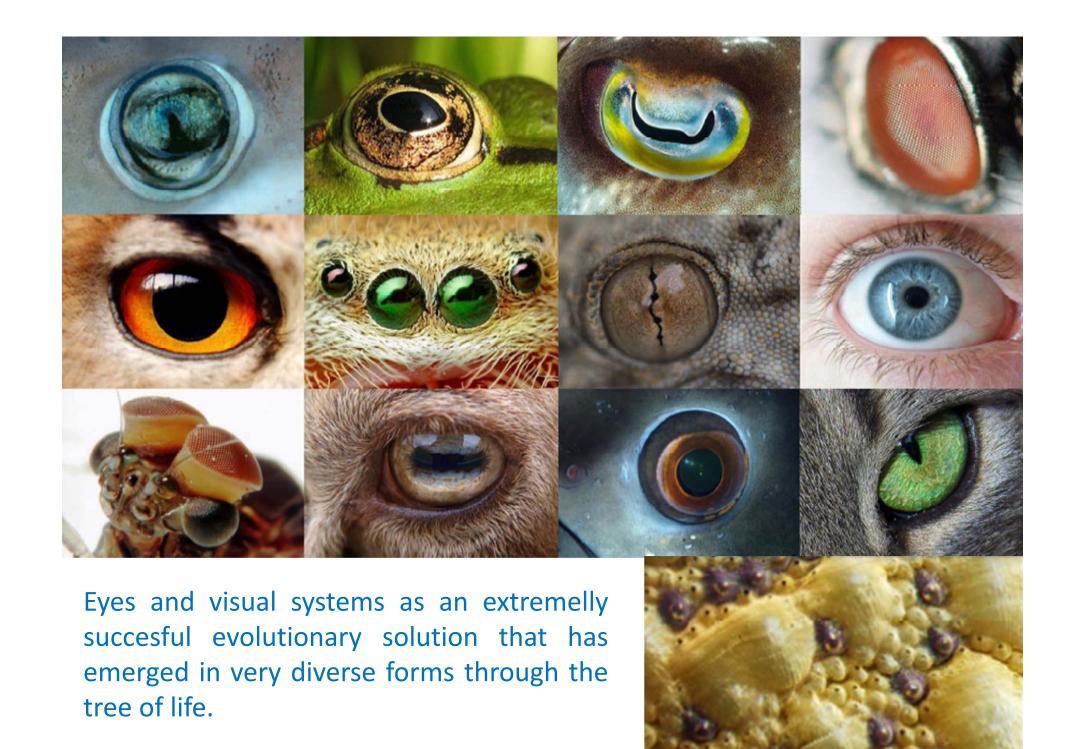


## Context as (pre)history

## Enter the Cambrian: A time of weapons and sensors

"From this point on, the mind evolved in response to other minds ..."



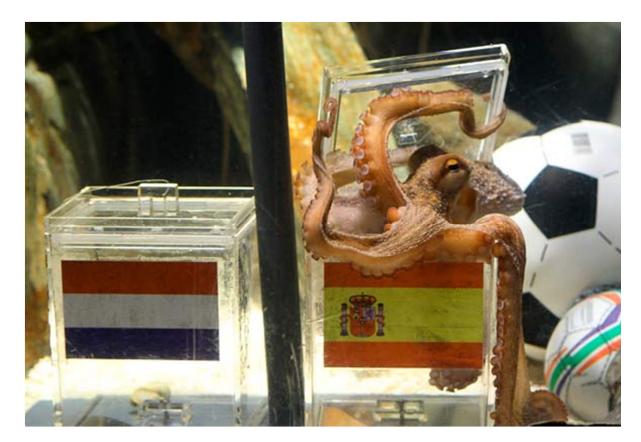


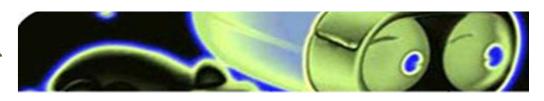


## Context as (pre)history

#### Meet the octopus

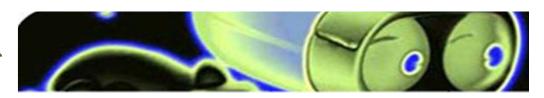
Departed from our branch in the evolutionary tree over 600M years ago and still it has evolved eyes not too dissimilar from ours (arguably better 'designed') and a large brain (Highest invertebrate brain-tobody mass ratio), not fully centralized (2/3 of neurons outside central brain; arms have "brains" of their own, with 10K+ neurons per suction cup) There is evidence that some of their 'relatives' are able to see through their skin (cuttlefish)





# **Bear that octopus in mind**





Evento

## EuroVis Invited Talk: Martin Wattenberg & Fernanda Viégas (Google)



Fecha+hora

Martes, 13 de junio de 2017 desde las 14:15 hasta las 15:40 (CEST) Ubicación

Open to members of UPC Auditori Vèrtex, UPC Campus Nord Barcelona España

Estado del pago

Pedido gratuito





# Wattenber and Viégas belong to the Big Picture (Data Visualization) Group

@ Google Brain

#### Their introductory talk title:

Visualization: The Secret Weapon of Machine Learning

#### Topics:

The TensorFlow Playground (see next slide)

How to scale visualization to DL?

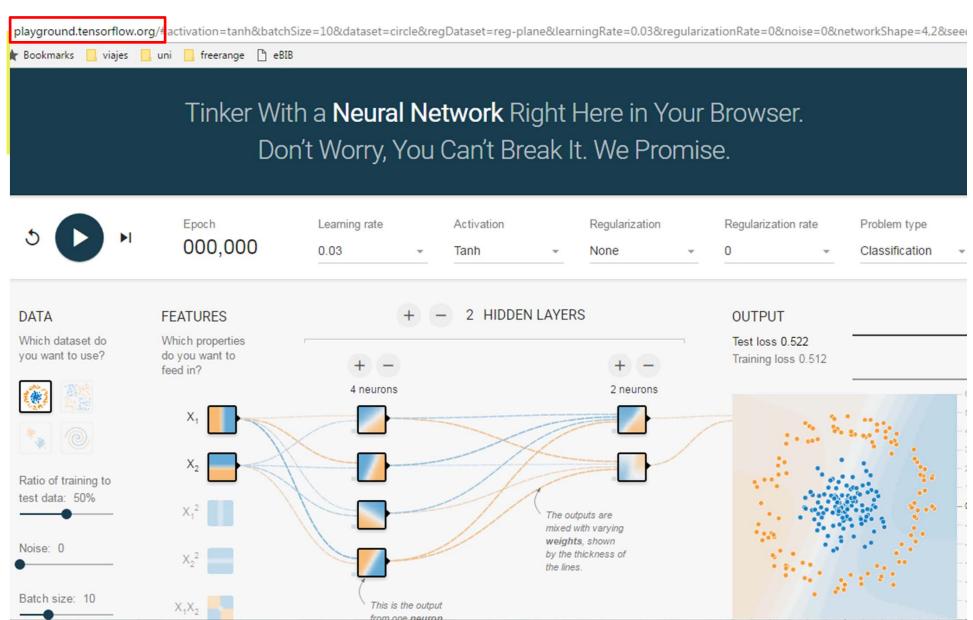
How to explain ANN decisions to end users?

Different end users:  $\leftarrow$  ML expert ... Final user  $\rightarrow$ 

Can we automate visualization to show relevant features?

Right level of complexity to show?







# The Big Picture (Data Visualization) Group

@ Google Brain

Visualization: The Secret Weapon of Machine Learning Their unsupervised weapon (see next slide):

projector.tensorflow.org

High dim spaces?

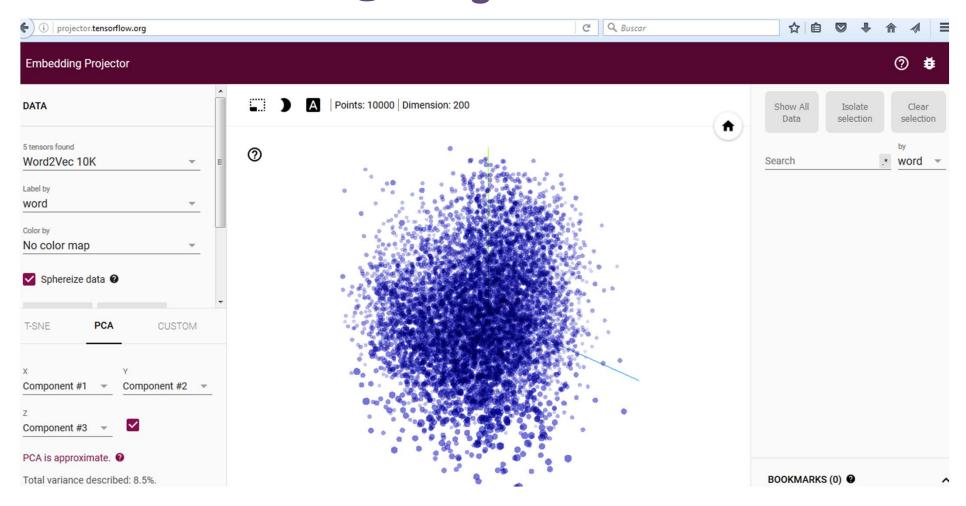
Right model to project?

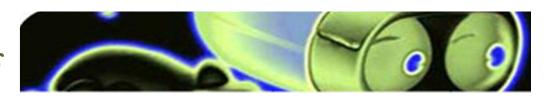
PCA & t-SNE

Too much to show?



# The Big Picture (Data Visualization) Group @ Google Brain





#### Interpretability just in recent conferences in BCN

### NIPS, ICANN, EuroVIS

## Interpretable ML for Complex Systems NIPS 2016 Workshop

About Call for Papers Invited Talks Organizers Program Committee Schedule

#### Interpreting the structure and predictions of complex models

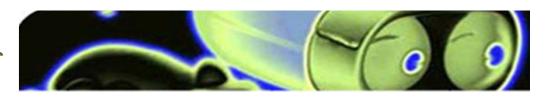
Complex machine learning models, such as deep neural networks, have recently achieved great predictive successes for visual object recognition, speech perception, language modeling, and information retrieval. These predictive successes are enabled by automatically learning expressive features from the data. Typically, these learned features are a priori unknown, difficult to engineer by hand, and hard to interpret. This workshop is about interpreting the structure and predictions of these complex models.

Interpreting the learned features and the outputs of complex systems allows us to more fundamentally understand our data and predictions. and to build more effective models. For example, we may build a complex model to predict long range crime activity. But by interpreting the learned structure of the model, we can gain new insights into the processing driving crime events, enabling us to develop more effective public policy. Moreover, if we learn, for example, that the model is making good predictions by discovering how the geometry of clusters of crime events affect future activity, we can use this knowledge to design avan mara euccaseful pradictiva modale



Key Dates

Workshop: 10 Dec 2016



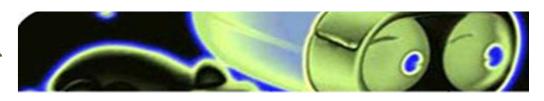
#### Interpretability just in recent conferences in BCN

ICANN16

25th International Conference on Artificial Neural Networks



**Workshop on Machine Learning and Interpretability** 



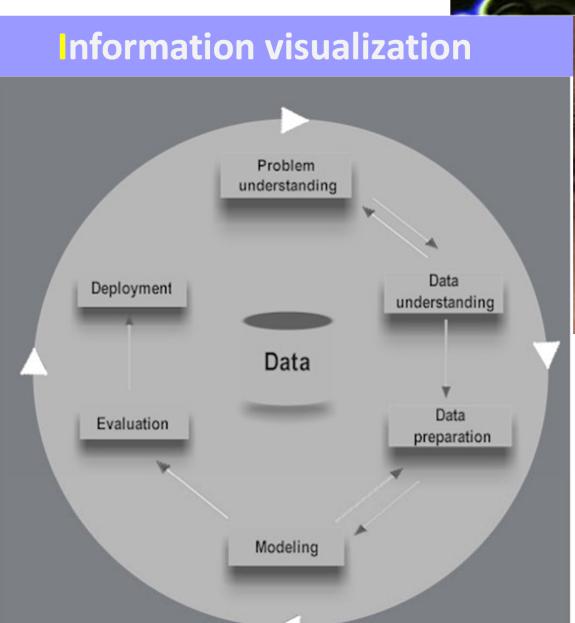


## Comprehensibility and Explanation in AI and ML

cex 2017

Quite frequently demands for better comprehensible and explainable Artificial Intelligence (AI) and Machine Learning (ML) systems are being put forward. The **cex** workshop sheds light on notions such as "comprehensibility" and "explanation" in the context of AI and ML, working towards a better understanding of what an explanation is when talking about intelligent systems, what it means to comprehend a system and its behaviour, and how human-machine interaction can take these dimensions into account.

The cex workshop will be held at the 16th International Conference of the Italian Association for Artificial Intelligence (AI\*IA 2017).





Arguably, we can locate info/data visualization and visual analytics in different places of the data analysis cycle: data understanding (through visual exploration), data preparation (feature extraction, for instance, can be visualization oriented), and/or data modeling (linear/nonlinear data visualization models)



#### Information visualization

- We aim discover the main characteristics of usually complex multivariate data sets, helping bring important aspects of the data into focus (think attention) for study in subsequent phases of the analysis.
- The task of data visualization is central to both data exploration and model interpretation.
- Adequate data visualizations can help us to gain insights into a problem without the frame of a conjecture: Out of a deductive model of research to reap the benefits of a more inductive one.
- ► The problem of knowledge generation through data visualization, is not circumscribed to data science *per se*. It can be addressed from the viewpoints of <u>both</u> artificial pattern recognition (APR) <u>and</u> natural pattern recognition (NPR).



#### **Information visualization**

# Artificial pattern recognition (APR):

Through the definition of methods /techniques /algorithms for data pre-processing and visualization.



► IV/VA defines processes that unify <u>DR algorithms</u> and visual user (interactive) interfaces to allow us to explore data and interpret models using graphical metaphors, in a way that helps to circumvent some of the inherent limitations of human vision.

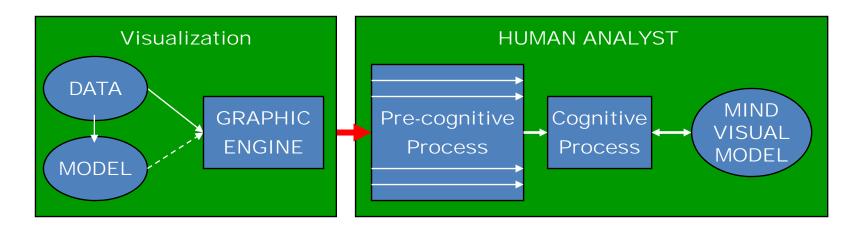
# Natural pattern recognition (NPR):

Understanding
visualization as the
cognitive processing of
visual stimuli conducted
by the human brain

Humans are equipped with visual NPR as a tool to understand the patterns of their natural environment and operate upon it.



#### Information visualization



**Pre-cognitive processing:** jigsaw pieces, or the interaction of visual elements put together by the brain's own data pre-processing.

**Visualization vs. mental model:** visual patterns, illusions and *Gestalt* laws.

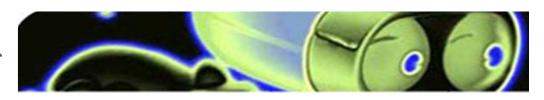
**Perception vs. sensation:** "It may often be rather hard to say how much from perceptions as derived from the sense of sight is due directly to sensation, and how much of them, on the other hand, is due to experience and training" **Hermann von Helmholtz, 1860 (Pollen, 1999, Cerebral Cortex)** 



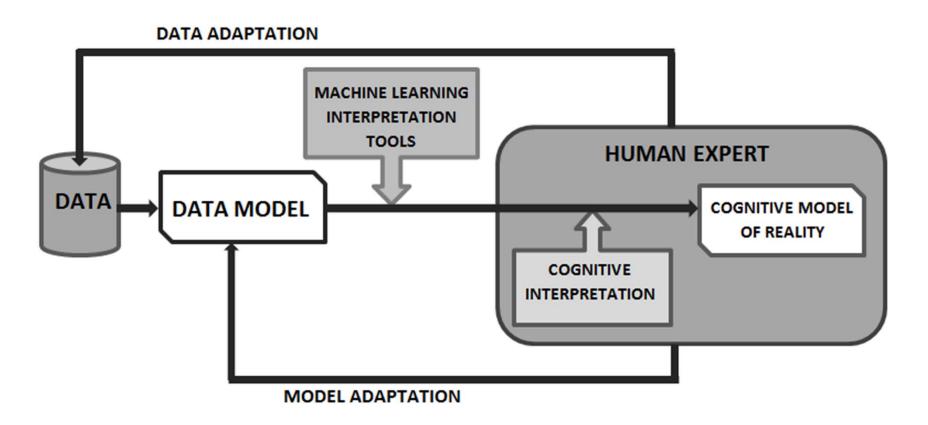
## nformation visualization



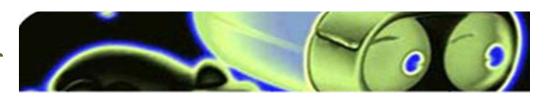




#### The human factor



• In the end, interpretability is a paramount quality that ML and related methods should aim to achieve if they are to be applied in practice.



#### So we <u>need</u> a formal framework for visualization

Lucky us, help is on its way



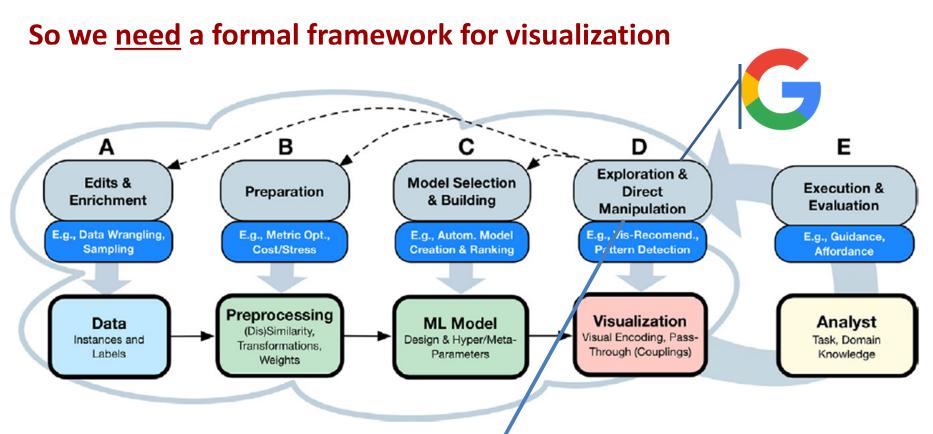
#### Neurocomputing

journal homepage: www.elsevier.com/locate/neucom

What you see is what you can change: Human-centered machine learning by interactive visualization

Dominik Sacha<sup>a,\*</sup>, Michael Sedlmair<sup>b</sup>, Leishi Zhang<sup>c</sup>, John A. Lee<sup>d</sup>, Jaakko Peltonen<sup>e</sup>, Daniel Weiskopf<sup>f</sup>, Stephen C. North<sup>g</sup>, Daniel A. Keim<sup>a</sup>



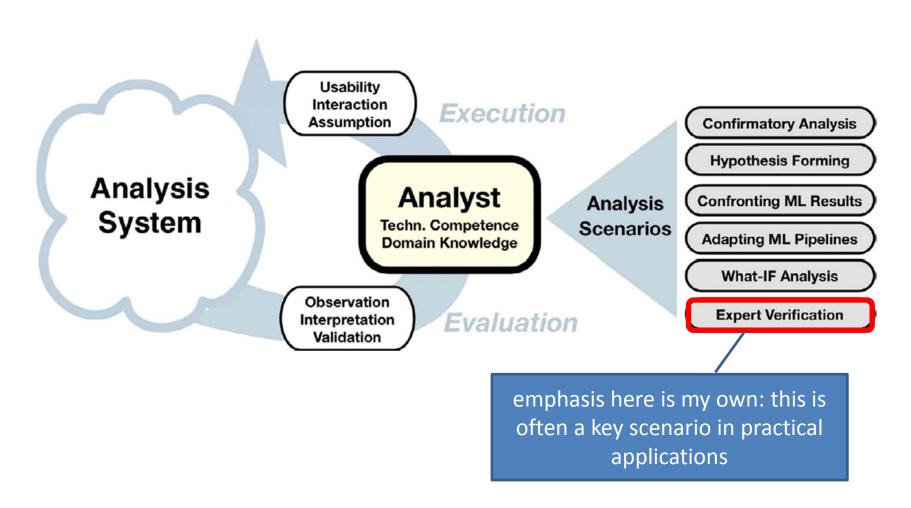


Aupetit M, Sedlmair M (2016) *SepMe: 2002 new visual separation measures*, *In Procs. of the IEEE Pacific Visualization Symposium*, 1–8.



#### So we need a formal framework for visualization

Lucky us, help is on its way

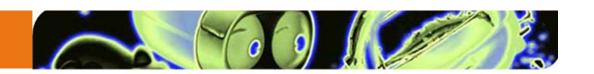


# HUMANS, INTERPRETABILITY, BIO- & HEALTH

# BIG DATA

## How big is yours? ... (2013, KDNuggets)

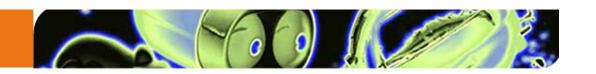
What was the largest dataset you analyzed / data mined? [322 votes]	
less than 1 MB (12)	3.7%
1.1 to 10 MB (8)	2.5%
11 to 100 MB (14)	4.3%
101 MB to 1 GB (50)	15.5%
1.1 to 10 GB (59)	18%
11 to 100 GB (52)	16%
101 GB to 1 Terabyte (59)	18%
1.1 to 10 TB (39)	12%
11 to 100 TB (15)	4.7%
101 TB to 1 Petabyte (6)	1.9%
1.1 to 10 PB (2)	0.6%
11 to 100 PB (0)	0%
over 100 PB (6)	1.9%



#### Some fun facts:

- Google processes over 20 PB worth of data every day.
- Back in December 2007, YouTube generated 27 PB of traffic.
- The CERN Large Hadron Collider (HLC) generetes about 20 PB of usable data per year.
- The volume of global annual data traffic is expected exceed 60,000 PB in 2016, from 8,000 petabytes in 2011
- In the next decade, astronomers expect to be processing 10 PB of data every hour from the Square Kilometre Array (SKA) telescope ➤ one exabyte every four days.

#### The Big Data Interpretation Challenge



# OK, but this is about the big ITCorps, la US NSA and the like, isn't it? ... or maybe not ...

**Nov 14** 

FOCUS ON BIG DATA



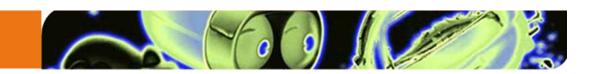
## nature neuroscience

# Focus on big data

Nature Neuroscience presents a special focus issue highlighting big data efforts under way in the field.

he number of big data projects in neuroscience, such as the BRAIN initiative in the United States or the Human Brain Mapping initiative in Europe, has been increasing in recent years. Will such big data efforts become the modus operandi in neuroscience, replacing smaller scale, hypothesis-driven science? How much insight will be gained from such projects? What are the best ways to go about conducting such

studies of the connectivity and activity of neurons seek to understand the relationship between these neural data and behavior. On page 1455, Alex Gomez-Marin and colleagues review technological advances that have accelerated the collection and analysis of big behavioral data, but argue that substantial challenges remain in interpreting the results of such efforts. They conclude that large-scale quantitative and open behavioral



# OK, but this is about the big ITCorps, la US NSA and the like, isn't it? ... or maybe not ...

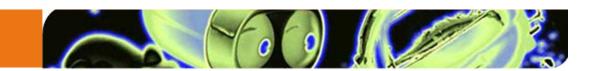
NATURE | TECHNOLOGY FEATURE

## Biology: The big challenges of big data

Vivien Marx

Nature 498, 255–260 (13 June 2013) doi:10.1038/498255a

Published online 12 June 2013



# OK, but this is about the big ITCorps, la US NSA and the like, isn't it? ... or maybe not ...

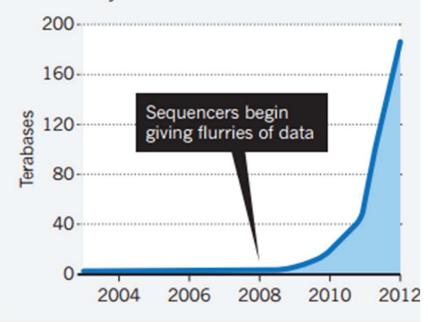
- Some extracts from the latter reference:
- "Biologists are joining the big-data club. With the advent of high-throughput genomics, life scientists are starting to grapple with massive data sets, encountering challenges with **handling**, **processing** and **moving** information that were once the domain of astronomers and high-energy physicists."
- "The European Bioinformatics Institute (EBI) in Hinxton, UK, [...] one of the world's largest biology-data repositories, currently stores 20 petabytes [...] Genomic data account for 2 Pb of that, a number that more than doubles every year."

# OK, but this is about the big ITCorps, la US NSA and the like, isn't it? ...

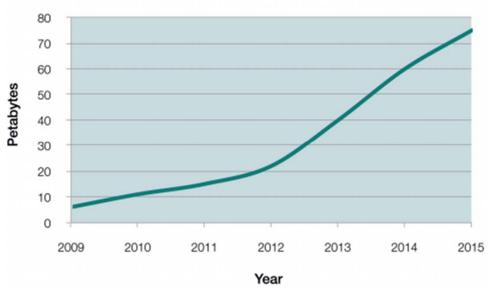
# DATA EXPLOSION The amount of genetic at the European Bioinfo

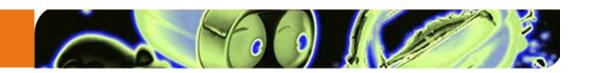
SOURCE: EMBL-EBI

The amount of genetic sequencing data stored at the European Bioinformatics Institute takes less than a year to double in size.



#### Total disk storage at EMBL-EBI





# OK, but this is about the big ITCorps, la US NSA and the like, isn't it? ...

\*\*Most researchers tend to download remote data to local hardware for analysis. But this method is "backward", says Andreas Sundquist, chief technology officer of DNAnexus. "The data are so much larger than the tools, it makes no sense to be doing that." The alternative is to use the cloud for both data storage and computing [...] There's no reason to move data outside the cloud. You can do analysis right there ..."

which would fit some of these guys' proposals ... FuroVis Invited Talk: Martin Wattenberg & Fernanda Viégas (Google)



Fecha+hora

Evento

Martes, 13 de junio de 2017 desde las 14:15 hasta las 15:40 (CEST) Ubicación

Open to members of UPC Auditori Vèrtex, UPC Campus Nord Barcelona España

Estado del pago
Pedido gratuito

# **SMALL DATA**

(more common than not)



## HUMANS, INTERPRETABILITY, BIO- & HEALTH

#### Data keep coming, which challenges attached:

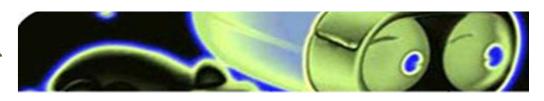
Extreme data heterogeneity

Multiple scales and multi-modality

Imbalance sample size  $\leftarrow \rightarrow$  dimensionality

SM Reza, Transforming Big Data into Computational Models for Personalized Medicine and Health Care, Dialogues in Clinical Neuroscience, **2016**, 18(3): 339-343

"Health care systems generate a huge volume of different types of data. Due to the complexity and challenges inherent in studying medical information, it is not yet possible to create a comprehensive model capable of considering all the aspects of health care systems. There are different points of view regarding what the most efficient approaches toward utilization of this data would be."



## HUMANS, INTERPRETABILITY, BIO- & HEALTH

Massive gaps between info / patterns / knowledge / decision making

#### Machines learn, doctors decide

"Machine Learning employed in healthcare will act as a tool to aid and refine specific tasks performed by human professionals"

MJ Reid, Black-Box Machine Learning: Implications for Healthcare, Polygeia, April 6, 2017



# HUMANS, INTERPRETABILITY, BIO- & HEALTH

#### Biomedical data analysis in translational research

Bhanot, Gyan; Biehl, Michael; Villmann, Thomas; Zühlke, Dietlind

#### Published in:

25th European Symposium on Artificial Neural Networks, Computational Intelligence and Machine Learning, FSANN 2017

# Authors highlight research questions & problems in Biomedicine & ML:

Analysis of structured, inhomogeneous and multimodal data

Feature selection and biomarker detection

Diagnosis and classification



# HUMANS, INTERPRETABILITY, BIO- & HEALTH

#### Biomedical data analysis in translational research

Bhanot, Gyan; Biehl, Michael; Villmann, Thomas; Zühlke, Dietlind

# Visualization & visual analytics (!)

- (a) Which visualization techniques are most suitable for heterogeneous and structured data in the biomedical context? How can we visualize relevant features in order to facilitate their interpretation by human experts?
- (c) How can one design feedback loops that can improve visualization models by integrating requirements/limitations of domain experts with the model?
- (d) How can we effectively visualize patient monitoring and critical events in a longitudinal assessment of patients?
- (e) How can we usefully display the errors/uncertainties resulting e.g. from embedding high-dimensional data into low dimensional spaces? Can these be visualized in an intuitive way?

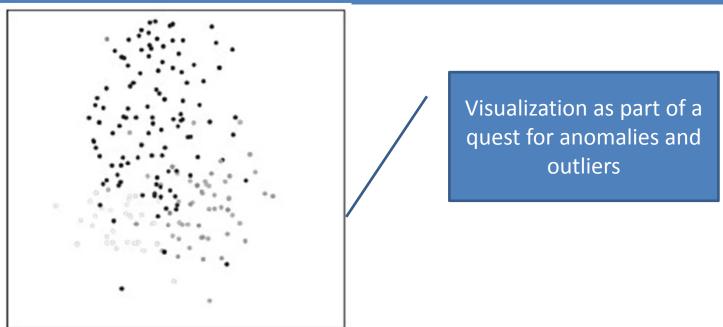


# Some examples from my own research: Who is the customer?

An example in the medical domain. Interpretation can also be a matter
of shared language. We could be talking in a different language that
domain experts might not be interested to talk.

# Brain tumour diagnosis for radiologists:

Vellido, A., Romero, E., González-Navarro, F.F., Belanche-Muñoz, Ll., Julià-Sapé, M., Arús, C. (2009) Outlier exploration and diagnostic classification of a multi-centre 1H-MRS brain tumour database. *Neurocomputing*, 72(13-15), 3085-3097.





# Some examples from my own research: Who is the customer?

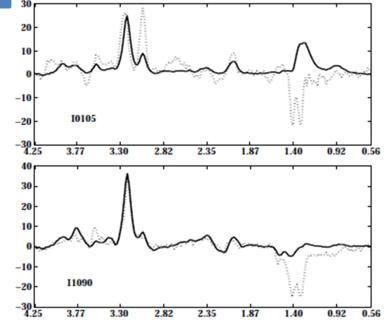
An example in the medical domain. Radiologists did not consider as outliers
many of the cases that our machine learning considered as such. Why? because as
humans they were still capable of identifying and characterizing such cases
without ambiguity.

# **Brain tumour diagnosis for radiologists:**

Vellido, A., Romero, E., González-Navarro, F.F., Belanche-Muñoz, Ll., Julià-Sapé, M., Arús, C. (2009) Outlier exploration and diagnostic classification of a multi-centre 1H-MRS brain tumour database. *Neurocomputing*, 72(13-15), 3085-3097.

#### Beware of prior expert knowledge

Id	Tum	Dis	Artifact-relat. outl.					
			noi	wat	ali	bas	pol	edd
I1061	G1(a2)				X			
I0062*	G2(gl)		X	X		X		
I0105*	G2(gl)	X						
I0172	G2(gl)			X		X		
I0175*	G2(gl)		X				X	
I0354*	G2(gl)			X			X	
I0428*	G2(gl)			X			X	



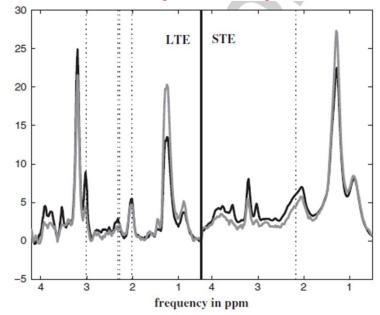


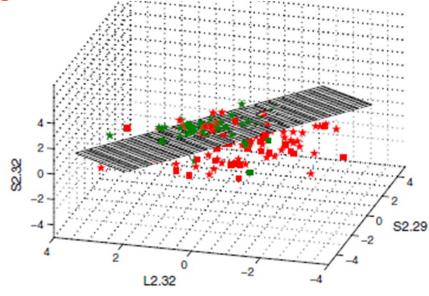
# Some examples from my own research: Who is the customer? (b)

- An example in the medical domain. Only the most straightforward 3-D visualization of a difficult classification problem finally convinced the medical experts of the relevance of our feature selection + classification results.
- Brain tumour diagnosis for radiologists:

Vellido, A., Romero, E., Julià-Sapé, M., Majós, C., Moreno-Torres, À., and Arús, C. (2012) Robust discrimination of glioblastomas from metastatic brain tumors on the basis of single-voxel proton MRS. *NMR in Biomedicine*, 25(6), 819-828.

Beware of prior expert knowledge







# Some examples from my own research: Who is the customer?

Another example from a different medical domain. Medical experts may only accept a
parsimonious outcome from a ML method, as they require an explainable basis for their
decision making that complies with their standard operational guidelines, often based on
simple and rigid attribute scores.

## Mortality prediction due to sepsis at the ICU:

Ribas, V.J., Vellido, A., Ruiz-Rodríguez, J.C., Rello, J. (2012) Severe sepsis mortality prediction with logistic regression over latent factors. *Expert Systems with Applications*, 39(2), 1937-1943.

- Only simple well-trodden models were accepted, despite better results being achieved with more sophisticated, less known models.
- Logistic Regression + Factor Analysis: as complex as it gets in an application context in which standard scores (SOFA, APACHE) are routinely used.
- Regardless success in prediction, end-user adoption of alternative methods should not be expected.
- Beware of existing methods of interpretation ...



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#### This is despite messages such as this:

"First, machine learning will dramatically improve prognosis. Current prognostic models (e.g., the Acute Physiology and Chronic Health Evaluation [APACHE] score and the Sequential Organ Failure Assessment [SOFA] score) are restricted to only a handful of variables, because humans must enter and tally the scores. But data could instead be drawn directly from EHRs or claims databases, allowing models to use thousands of rich predictor variables. Does doing so lead to better predictions?"

Z Obermeyer, EJ Emanuel (2016) New England Journal of Medicine, 375(13)



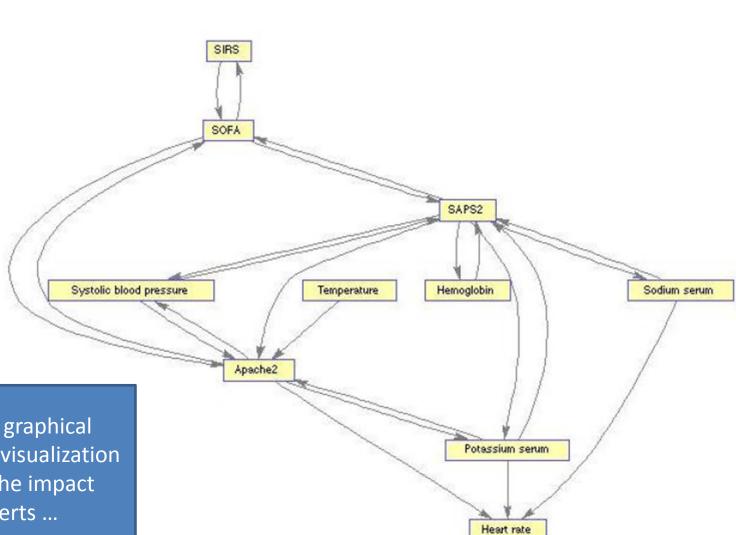
#### Who is the customer?

Another (
 parsimon
 decision (
 simple an)

# **Mortality**

Ribas, V.J., Ve prediction w 39(2), 1937-1

More complex graphical models and their visualization achieved half the impact among experts ...



# SIMPLE MODELS x SMALL DATA

This experience at least partially fits the viewpoint of "politically incorrect" Prof. David J. Hand

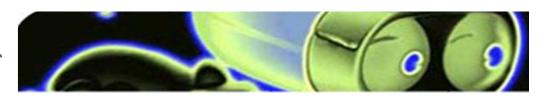
Statist. Sci. Volume 21, Number 1 (2006), 1-14.

# Classifier Technology and the Illusion of Progress

David J. Hand

#### **Abstract**

A great many tools have been developed for supervised classification, ranging from early methods such as linear discriminant analysis through to modern developments such as neural networks and support vector machines. A large number of comparative studies have been conducted in attempts to establish the relative superiority of these methods. This paper argues that these comparisons often fail to take into account important aspects of real problems, so that the apparent superiority of more sophisticated methods may be something of an illusion. In particular, simple methods typically yield performance almost as good as more sophisticated methods, to the extent that the difference in performance may be swamped by other sources of uncertainty that generally are not considered in the classical supervised classification paradigm.



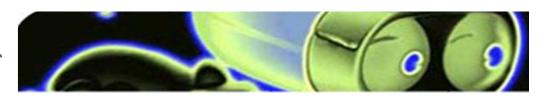
# Some general comments on DR for Interpretation

- Problems of high and very high dimensionality are becoming commonplace in bio-fields such as, for instance, bioinformatics ...
- Almost no problem is interpretable in practice if all data attributes are retained and used to provide an outcome. Furthermore, data of very high-dimensionality are bound to show unexpected geometrical properties that might affect their modeling and bias the interpretation of results.
- Two main DR approaches: feature selection (supervised and unsupervised) and feature extraction, in which new non-observable features are created on the basis of the observed ones ...
- NOTE: some of the <u>most popular</u> DR techniques in real-world applications are precisely <u>some of the simplest ones</u> (e.g., the ubiquitous PCA).



# Some general comments on (NL)DR for Interpretation

- Many relevant ML contributions to the problem of multivariate data DR have stemmed from the field of NLDR.
- The challenge of interpretability is very explicit here: NLDR methods rarely provide an easy interpretation of the outcome in terms of the original data features, because such outcome is usually a non-trivial nonlinear function of these features.
- NLDR techniques usually attempt to minimize the distortion they introduce in the mapping of the data from the observed space onto lower-dimensional spaces.



# (Yet) more help on the way ...

IEEE TRANSACTIONS ON VISUALIZATION AND COMPUTER GRAPHICS VOL. 23. NO. 1. JANUARY 2017

# Visual Interaction with Dimensionality Reduction: A Structured Literature Analysis

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# Wrap up

- The journey from data to knowledge is treacherous and knowledge discovery processes require model interpretation.
- ML & related models' users should aspire not only to integrate interpretation strategies ... but also to negotiate with end-users (very specially those in the medical and heath domains) the terms of that interpretability.
- NLDR models (and nonlinear models in general) are not likely to become mainstream in many app fields unless they are designed with interpretability in mind.
- Graphical metaphors (visualization, graphical models) are naturally suited as interpretability tools.
- When handling interpretability, we can only <u>ignore NPR</u> at our <u>own</u> <u>peril</u> and adding interactivity to the VA process could be (the?) key to succesful application.





# Some further reading

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- Condry, N (2016). Meaningful models: utilizing conceptual structure to improve Machine Learning interpretability. *arXiv* preprint arXiv:1607.00279.
- Doshi-Velez, F & Kim, B (2017) Towards a rigorous science of interpretable
   Machine Learning. arXiv:1702.08608v2
- Lipton, ZC (2017) The mythos of model interpretability. arXiv:1606.03490v3
- Goodman, B & Flaxman, S (2016) EU regulations on algorithmic decision-making and a "right to explanation". ICML Workshop on Human Interpretability in Machine Learning (WHI 2016), New York, NY. arXiv preprint arXiv:1606.08813.



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 Goodman, B & Flaxman, S (2016) EU regulations on algorithmic decision-making and a "right to explanation". arXiv preprint arXiv:1606.08813.

#### **Abstract**

Protection Regulation will have on the routine use of machine learning algorithms. Slated to take effect as law across the EU in 2018, it will restrict automated individual decision-making (that is, algorithms that make decisions based on user-level predictors) which "significantly affect" users. The law will also effectively create a "right to explanation", whereby a user can ask for an explanation of an algorithmic decision that was made about them. We argue that while this law will pose large challenges for industry, it highlights opportunities for computer scientists to take the lead in designing algorithms and evaluation frameworks which avoid discrimination and enable explanation.

