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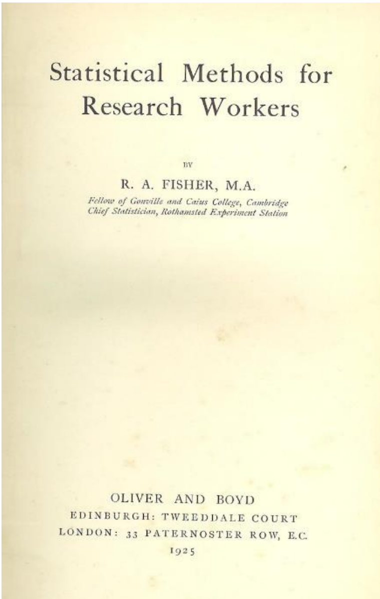
The data science revolution in scientific research

Jonathan Rowe
Programme Director, Data Science for Science



Statistical Methods for
Research Workers

BY

R. A. FISHER, M.A.

Fellow of Gonville and Caius College, Cambridge
Chief Statistician, Rothamsted Experiment Station

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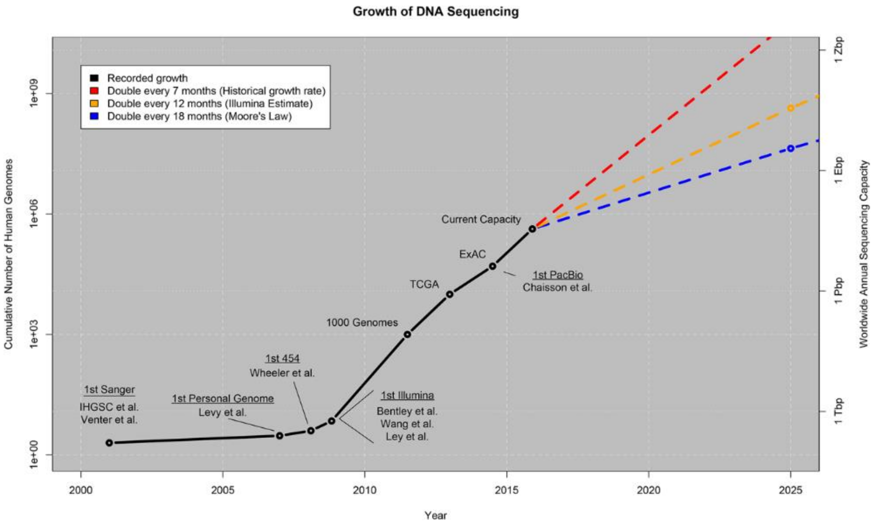

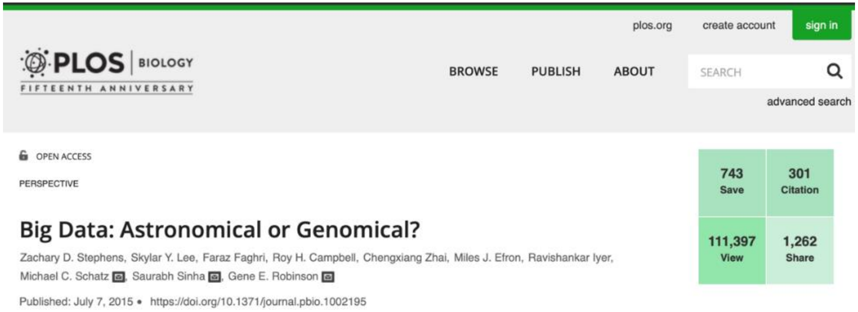

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Published: July 7, 2015 • https://doi.org/10.1371/journal.pbio.1002195

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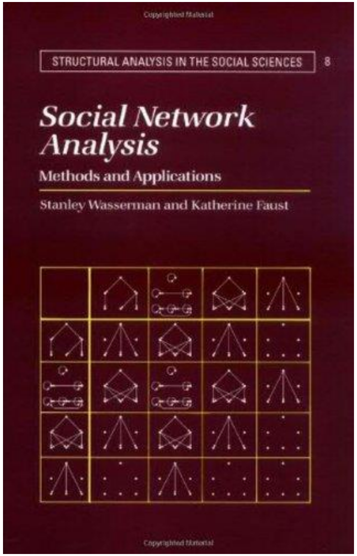
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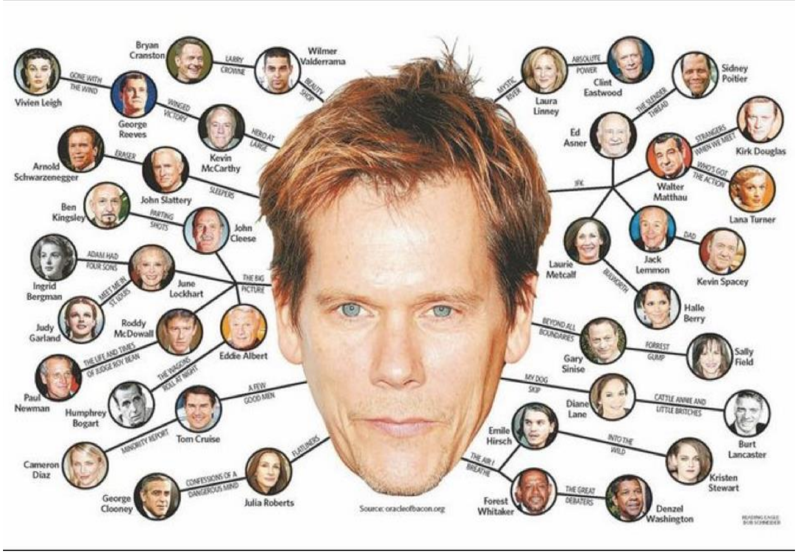
Social Network Analysis
Methods and Applications
Stanley Wasserman and Katherine Faust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RESEARCH ARTICLE

Testing for Questionable Research Practices in a Meta-Analysis: An Example from Experimental Parapsychology

Dick J. Bierman[1,2]*, James P. Spottiswoode[3], Aron Bijl[4]

1 Experimental Psychology, University of Groningen, Groningen, The Netherlands, **2** Brain & Cognition, University of Amsterdam, Amsterdam, The Netherlands, **3** LFR, Palo Alto, California, United States of America, **4** Brain & Cognition, University of Amsterdam, Amsterdam, The Netherlands

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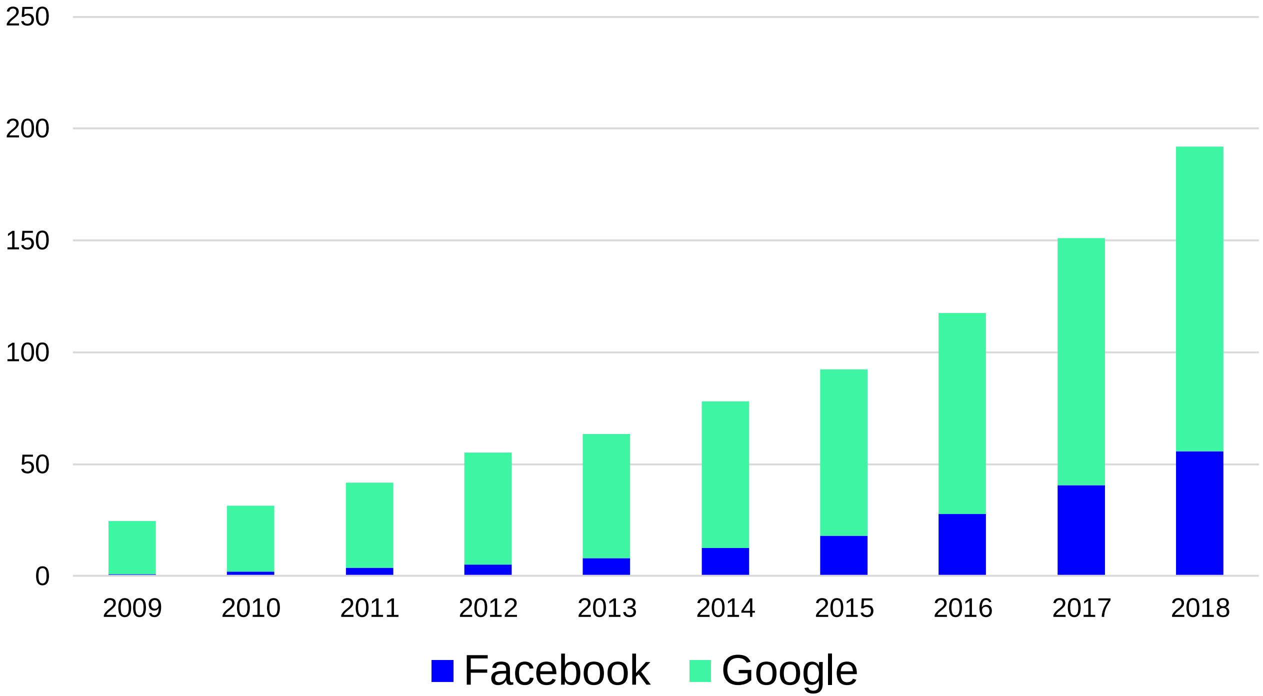

ImageNet Classification with Deep Convolutional Neural Networks

Alex Krizhevsky
University of Toronto
kriz@cs.utoronto.ca

Ilya Sutskever
University of Toronto
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Geoffrey E. Hinton
University of Toronto
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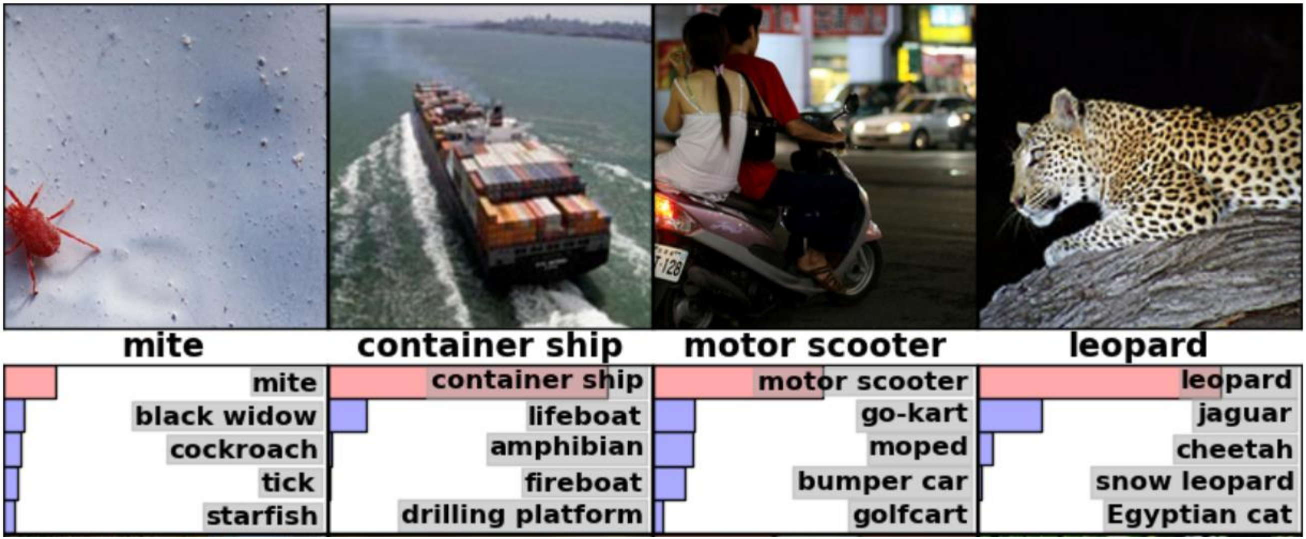
Abstract

We trained a large, deep convolutional neural network to classify the 1.2 million high-resolution images in the ImageNet LSVRC-2010 contest into the 1000 different classes. On the test data, we achieved top-1 and top-5 error rates of 37.5% and 17.0% which is considerably better than the previous state-of-the-art. The neural network, which has 60 million parameters and 650,000 neurons, consists of five convolutional layers, some of which are followed by max-pooling layers, and three fully-connected layers with a final 1000-way softmax. To make training faster, we used non-saturating neurons and a very efficient GPU implementation of the convolution operation. To reduce overfitting in the fully-connected layers we employed a recently-developed regularization method called "dropout" that proved to be very effective. We also entered a variant of this model in the ILSVRC-2012 competition and achieved a winning top-5 test error rate of 15.3%, compared to 26.2% achieved by the second-best entry.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container ship
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starfish
container ship
lifeboat
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fireboat
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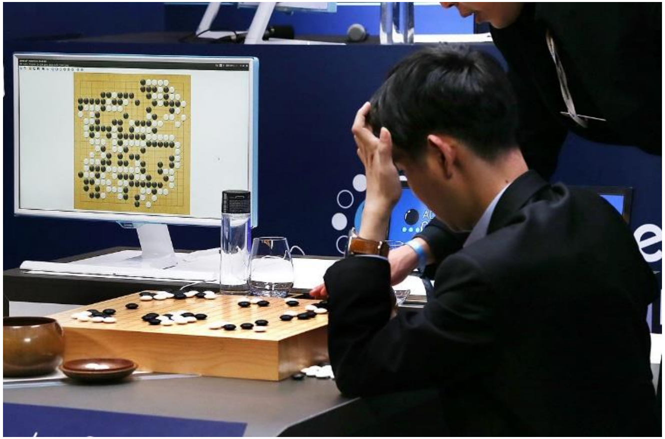
motor scooter
go-kart
moped
bumper car
golfcart
leopard
jaguar
cheetah
snow leopard
Egyptian cat

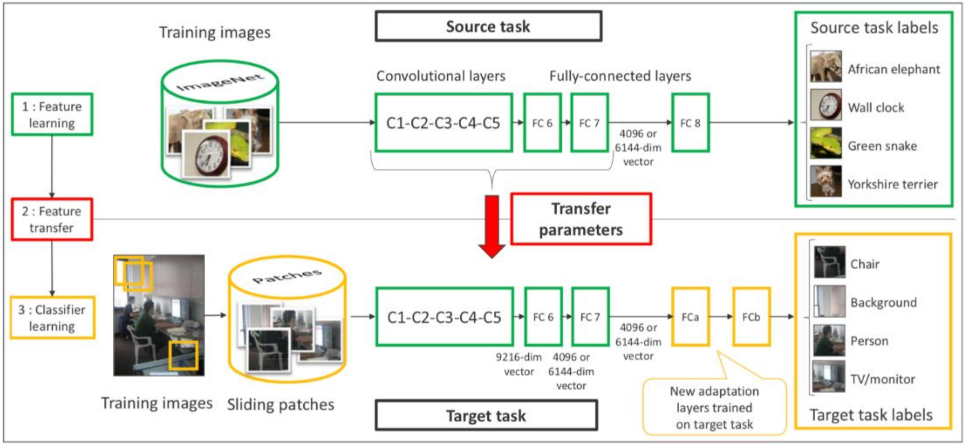

truck 0.959
person 0.968
tie 0.89
car 0.967
car 0.983
car 0.957
truck 0.940
truck 0.779
bicycle 0.761



A general reinforcement learning algorithm that masters chess, shogi and Go through self-play

David Silver,[1,2*] Thomas Hubert,[1*] Julian Schrittwieser,[1*]
Ioannis Antonoglou,[1,2] Matthew Lai,[1] Arthur Guez,[1] Marc Lanctot,[1]
Laurent Sifre,[1] Dharshan Kumaran,[1,2] Thore Graepel,[1,2]
Timothy Lillicrap,[1] Karen Simonyan,[1] Demis Hassabis[1]

[1]DeepMind, 6 Pancras Square, London N1C 4AG.
[2]University College London, Gower Street, London WC1E 6BT.



Learning and Transferring Mid-Level Image Representations using Convolutional Neural Networks

Maxime Oquab[1,*] Leon Bottou[2] Ivan Laptev[1,*] Josef Sivic[1,*]
[1]INRIA, Paris, France [2]MSR, New York, USA

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SCIENTIFIC REPORTS

Article | OPEN | Published: 16 October 2017

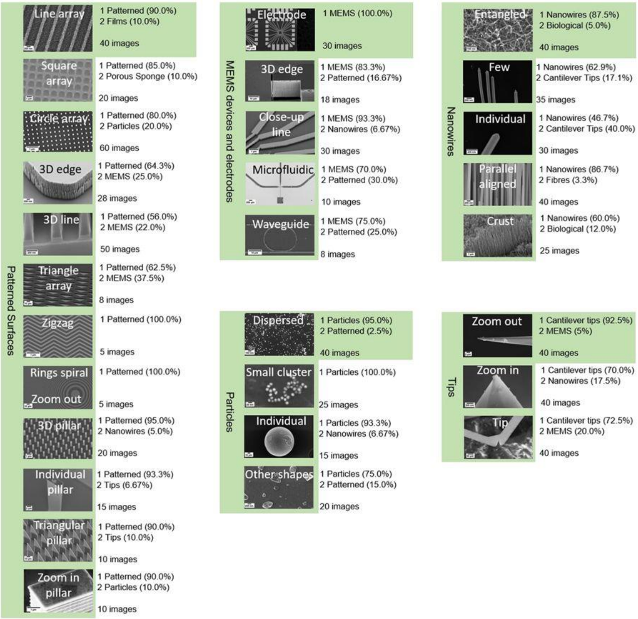
Neural Network for Nanoscience Scanning Electron Microscope Image Recognition

Mohammad Hadi Modarres, Rossella Aversa, Stefano Cozzini, Regina Ciancio, Angelo Leto & Giuseppe Piero Brandino

Scientific Reports **7**, Article number: 13282 (2017) | Download Citation

Abstract

In this paper we applied transfer learning techniques for image recognition, automatic categorization, and labeling of nanoscience images obtained by scanning electron microscope (SEM). Roughly 20,000 SEM images were manually classified into 10 categories to form a labeled training set, which can be used as a reference set for future applications of deep learning enhanced algorithms in the nanoscience domain. The categories chosen spanned the range of 0-Dimensional (0D) objects such as particles, 1D nanowires and fibres, 2D films and coated surfaces, and 3D patterned surfaces such as pillars. The training set was used to retrain on the SEM dataset and to compare many



Generative Adversarial Nets

Ian J. Goodfellow,* Jean Pouget-Abadie,† Mehdi Mirza, Bing Xu, David Warde-Farley, Sherjil Ozair,‡ Aaron Courville, Yoshua Bengio§
Département d'informatique et de recherche opérationnelle
Université de Montréal
Montréal, QC H3C 3J7

Published as a conference paper at ICLR 2018

Progressive Growing of GANs for Improved Quality, Stability, and Variation

Tero Karras NVIDIA
Timo Aila NVIDIA
Samuli Laine NVIDIA
Jaakko Lehtinen NVIDIA and Aalto University
{tkarras,taila,slaine,jlehtinen}@nvidia.com

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Accelerating Science with Generative Adversarial Networks: An Application to 3D Particle Showers in Multilayer Calorimeters

Michela Paganini, Luke de Oliveira, and Benjamin Nachman
Phys. Rev. Lett. **120**, 042003 – Published 26 January 2018

Article | References | Citing Articles (11) | PDF | HTML | Export Citation

ABSTRACT

Physicists at the Large Hadron Collider (LHC) rely on detailed simulations of particle collisions to build expectations of what experimental data may look like under different theoretical modeling assumptions. Petabytes of simulated data are needed to develop analysis techniques, though they are expensive to generate using existing algorithms and computing resources. The modeling of detectors and the precise description of particle cascades as they interact with the material in the calorimeter are the most computationally demanding steps in the simulation pipeline. We therefore introduce a deep neural network-based generative model to enable high-fidelity, fast, electromagnetic calorimeter simulation. There are still challenges for achieving precision across the entire phase space, but our current solution can reproduce a variety of particle shower properties while achieving speedup factors of up to $100\,000\times$. This opens the door to a new era of fast simulation that could save significant computing time and disk space, while extending the reach of physics searches and precision measurements at the LHC and beyond.

Active learning machine learns to create new quantum experiments

Alexey A. Melnikov, Hendrik Poulsen Nautrup, Mario Krenn, Vedran Dunjko, Markus Tiersch, Anton Zeilinger, and Hans J. Briegel

PNAS February 6, 2018 115 (6) 1221-1226; published ahead of print January 18, 2018 https://doi.org/10.1073/pnas.1714936115

Contributed by Anton Zeilinger, November 14, 2017 (sent for review August 24, 2017; reviewed by Jacob D. Biamonte and Jonathan P. Dowling)

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Significance

Quantum experiments push the envelope of our understanding of fundamental concepts in quantum physics. Modern experiments have exhaustively probed the basic notions of quantum theory. Arguably, further breakthroughs require the tackling of complex quantum phenomena and consequently require complex experiments and involved techniques. The designing of such complex experiments is difficult and often clashes with human intuition. We present an autonomous learning model which learns to design such complex experiments, without relying on previous knowledge or often flawed intuition. Our system not only learns how to design desired experiments more efficiently than the best previous approaches, but in the process also discovers nontrivial experimental techniques. Our work demonstrates that learning machines can offer dramatic advances in how experiments are generated.

Founding the Institute

"We will found The Alan Turing Institute to ensure Britain leads the way again in the use of big data and algorithm research"

George Osborne, Chancellor of the Exchequer
Budget Speech, March 2014

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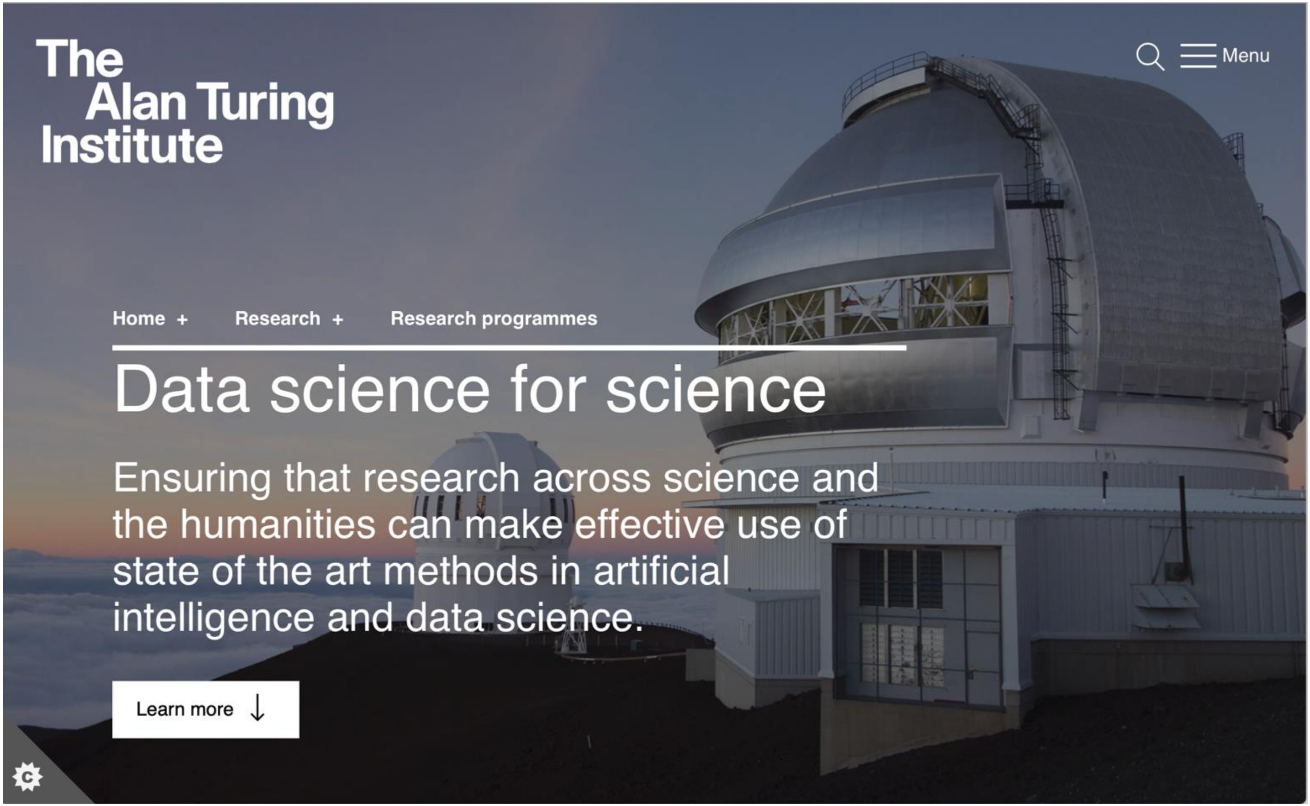
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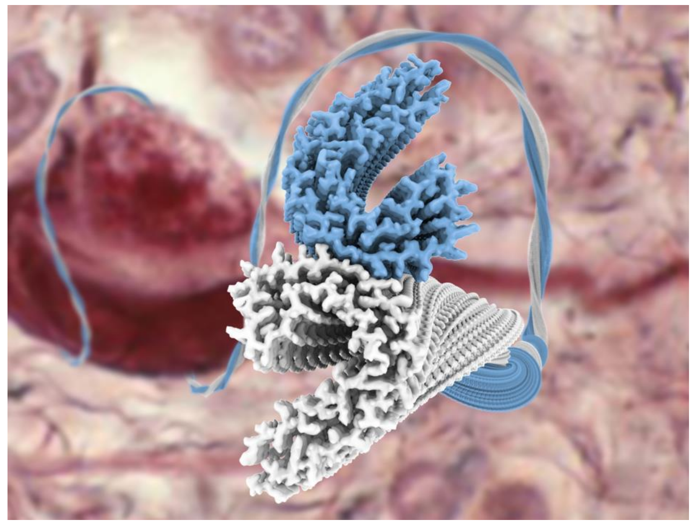
Article | Published: 05 July 2017

Cryo-EM structures of tau filaments from Alzheimer's disease

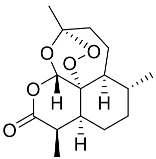
Anthony W. P. Fitzpatrick, Benjamin Falcon, Shaoda He, Alexey G. Murzin, Garib Murshudov, Holly J. Garringer, R. Anthony Crowther, Bernardino Ghetti, Michel Goedert & Sjors H. W. Scheres

Nature **547**, 185–190 (13 July 2017) | Download Citation



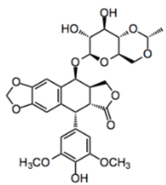
Anti-malarial

Artemisinin
Wormwood
(*artemisia annua*)



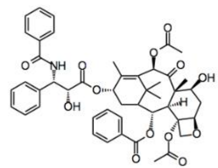
Anti-cancer

Etoposide Mayapple
(*podophyllum)*



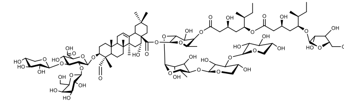
Anti-cancer

Taxol Yew
(*taxus baccata*)



Adjuvant

Qs-21 Soapbark
(*quillaja saponaria*)



The majority of plant natural products cannot be accessed – and most of them have not yet been discovered

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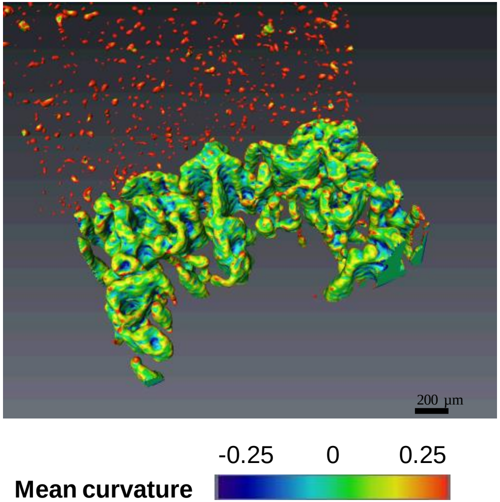

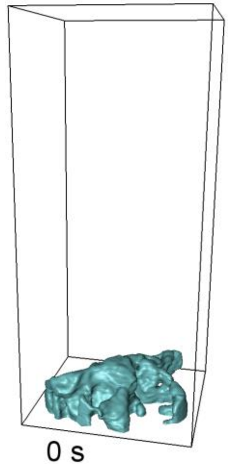

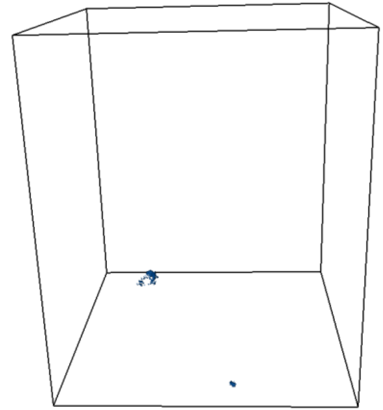

A positive mean curvature means concave towards the liquid

B. Cai et al. Acta Mater. 2014(76): 371-380; B. Cai et al. Acta Mater. 2017(117):160-169;
B. Cai et al. Scripta Mater. submitted.

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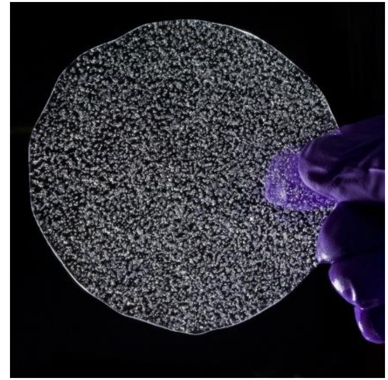

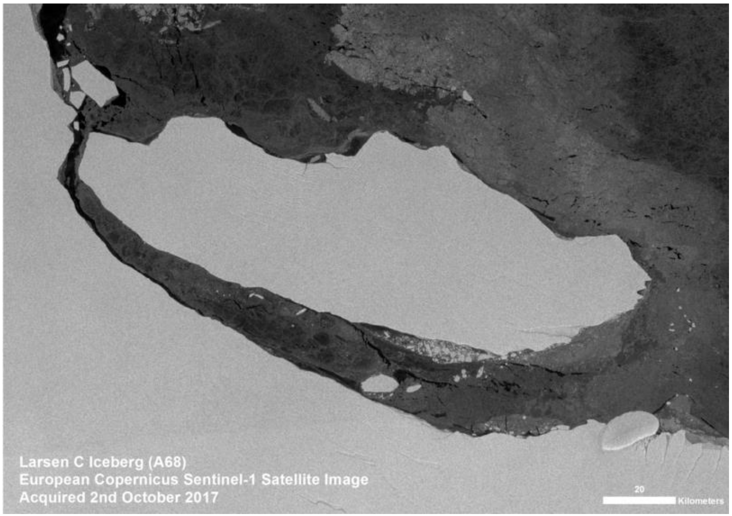

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Francisco de Goya, Doña Isabel de Porcel (NG1473), before 1805

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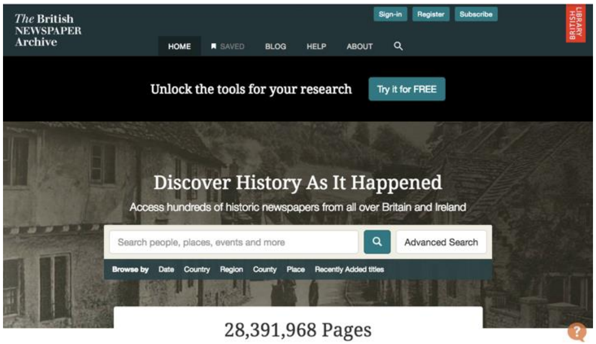

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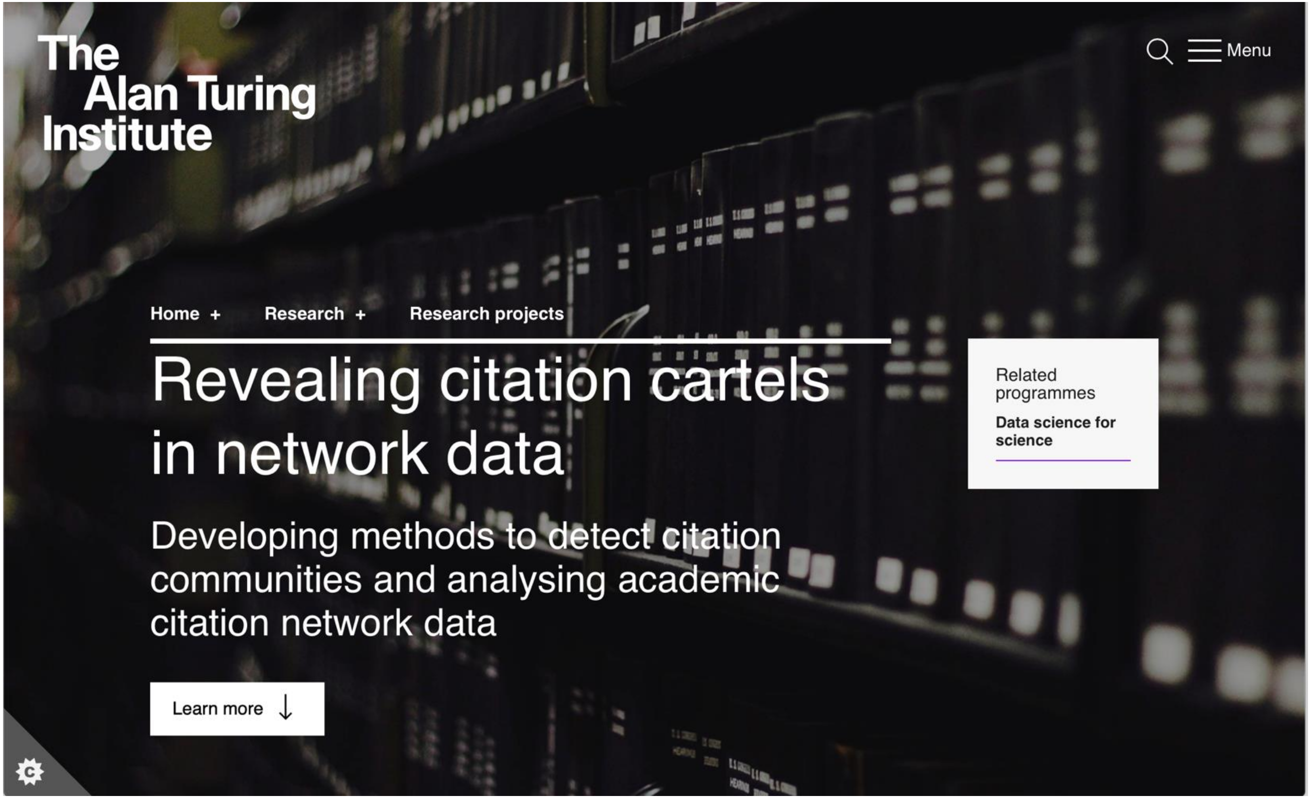
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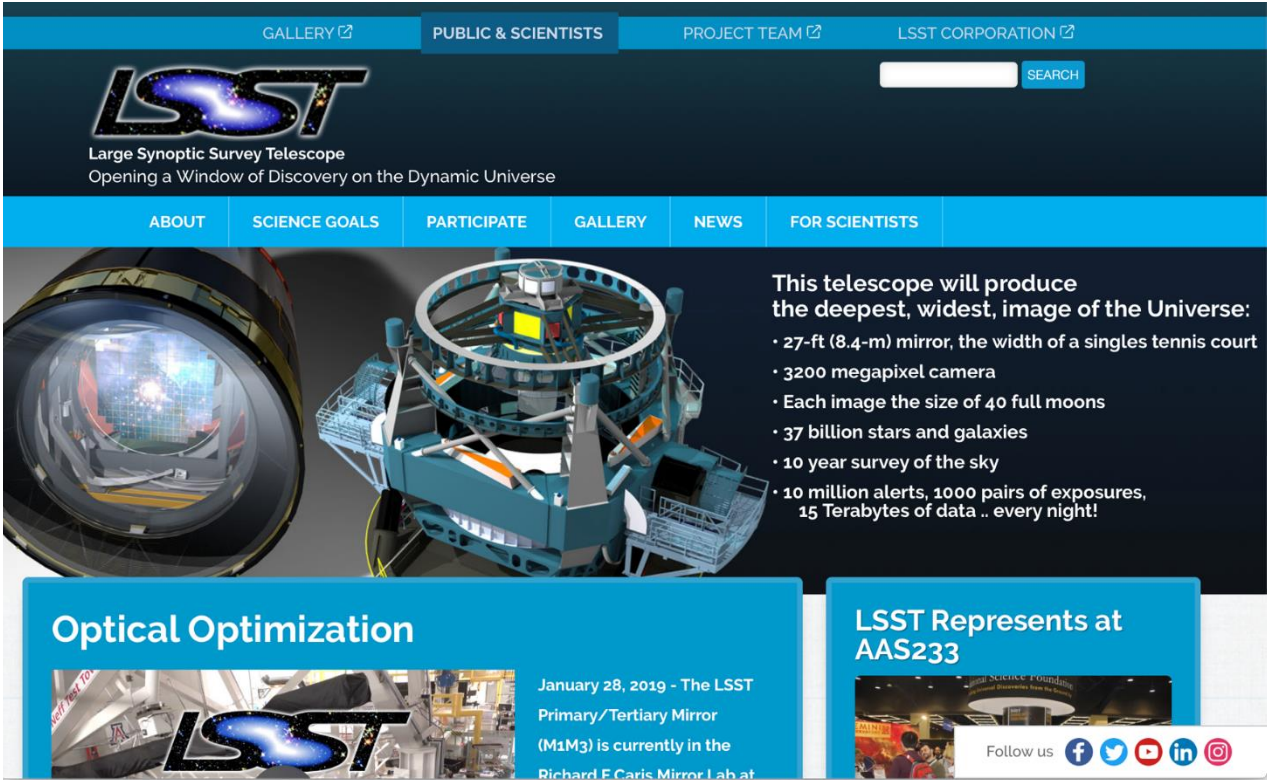
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• 10 year survey of the sky
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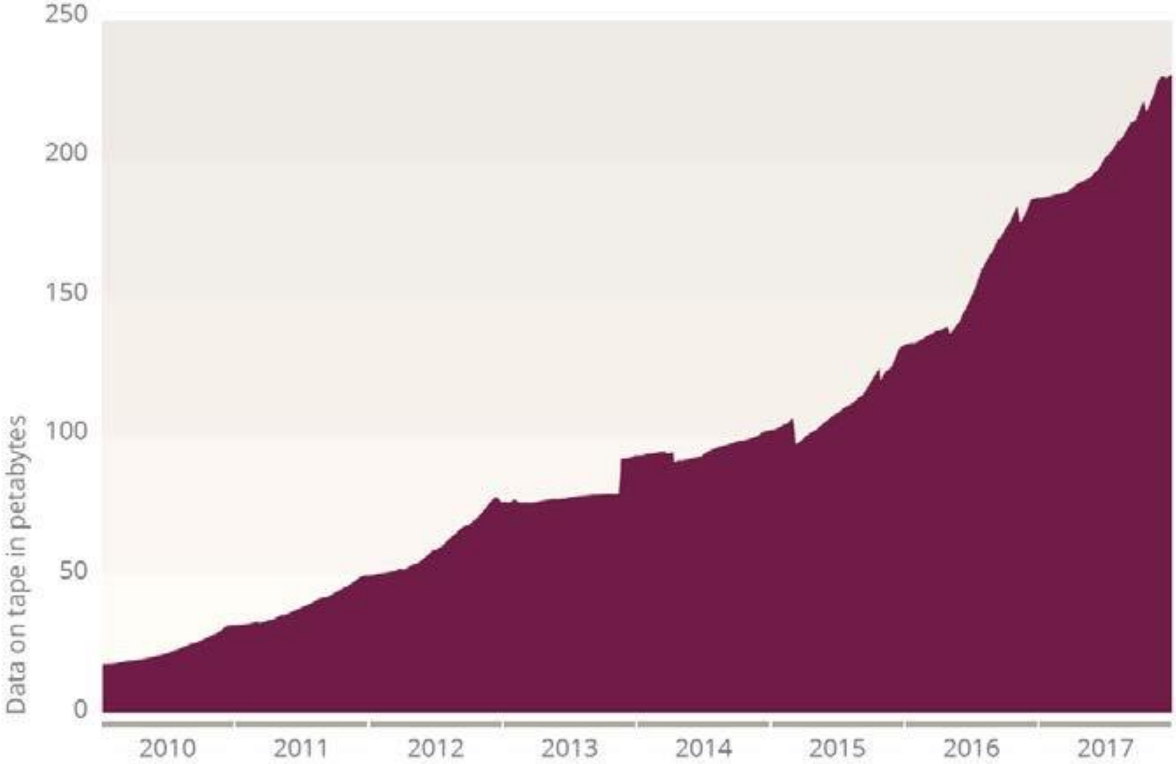
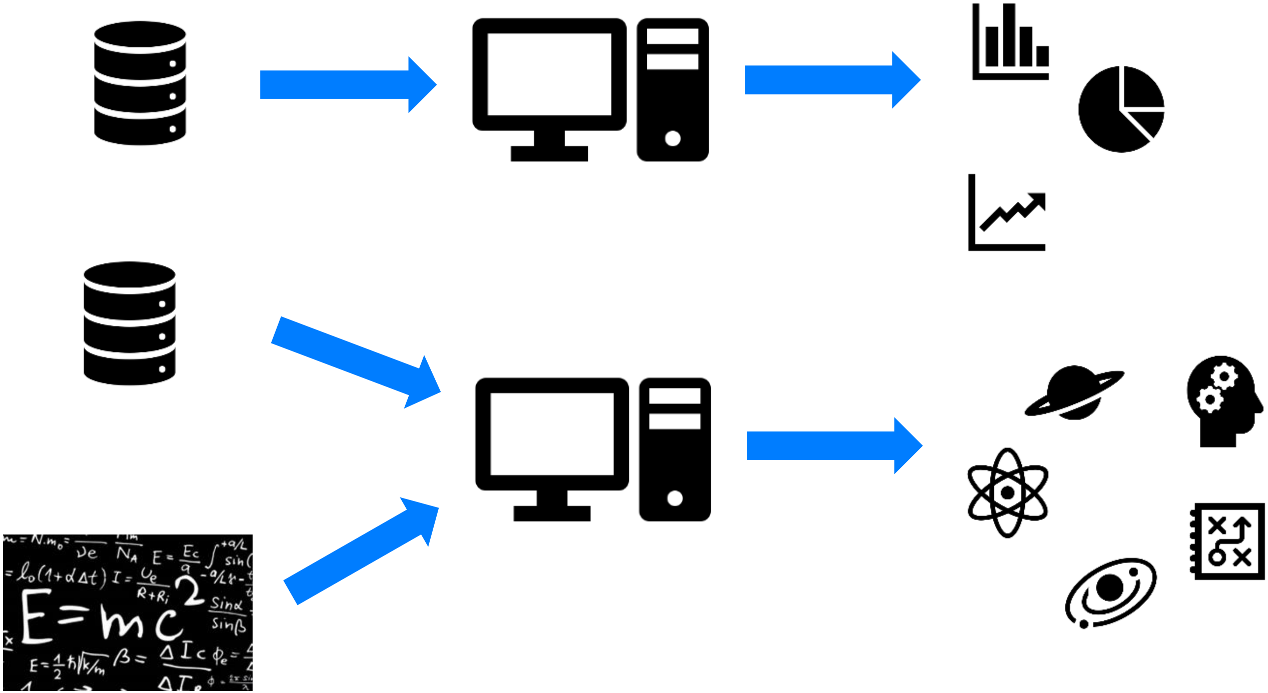


"A just machine to make big decisions
Programmed by fellows with compassion and vision
We'll be clean when their work is done
We'll be eternally free, yes and eternally young.

What a beautiful world this will be
What a glorious time to be free."

Donald Fagen
I.G.Y. (International Geophysical Year)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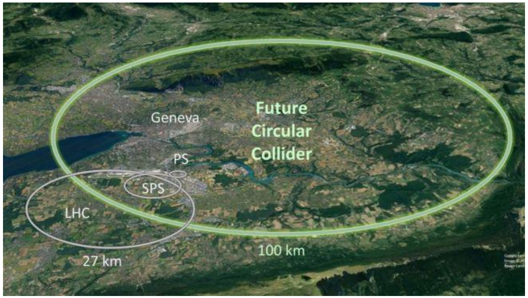
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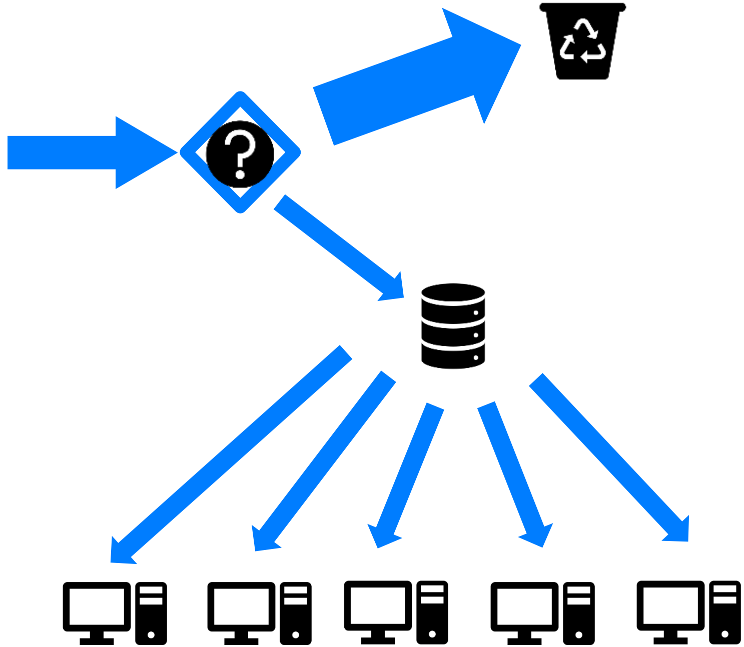
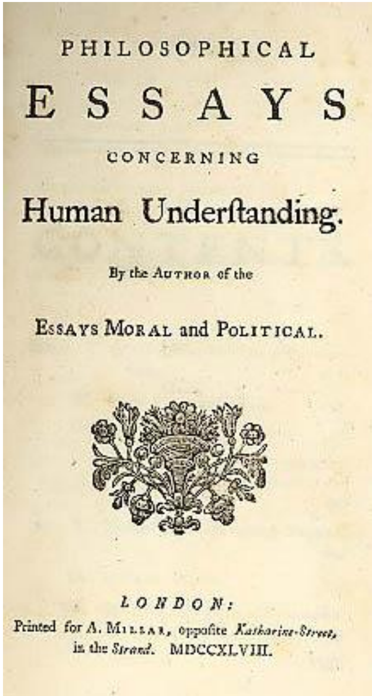
SPS
LHC
27 km
100 km





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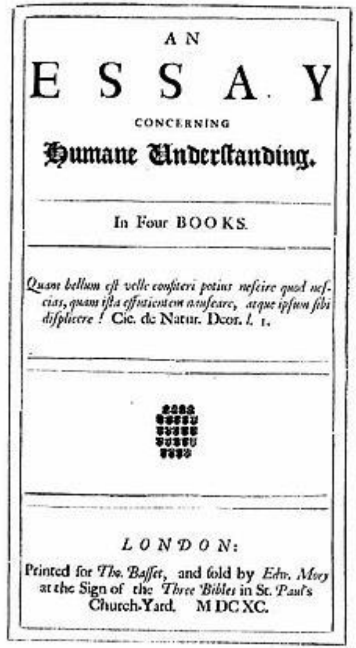

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der

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von

Immanuel Kant

Profeſſor in Königsberg.

Riga,

verlegts Johann Friedrich Hartknoch

1781.

RESEARCH | *REPORTS*

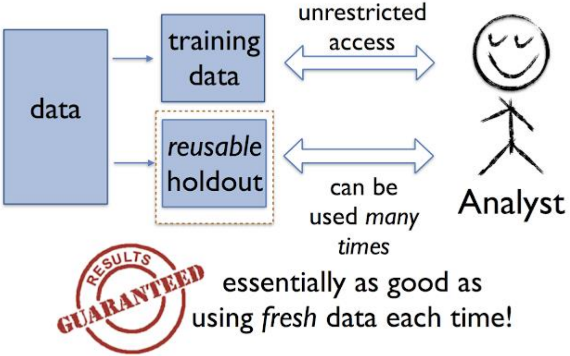
STATISTICS

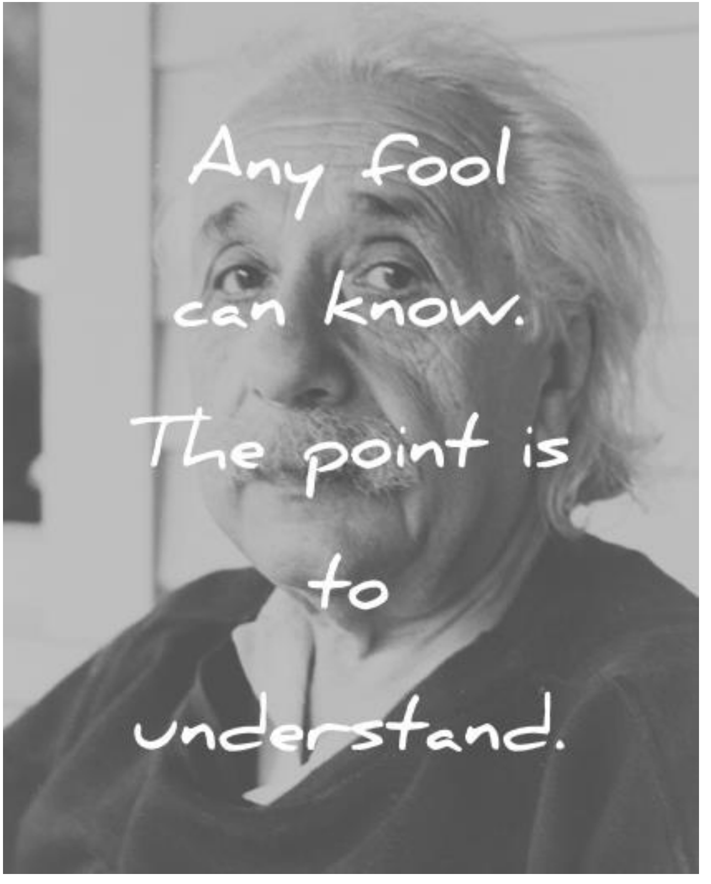
The reusable holdout: Preserving validity in adaptive data analysis

Cynthia Dwork,[1*] Vitaly Feldman,[2*] Moritz Hardt,[3*] Toniann Pitassi,[4*] Omer Reingold,[5*] Aaron Roth[6*]

Misapplication of statistical data analysis is a common cause of spurious discoveries in scientific research. Existing approaches to ensuring the validity of inferences drawn from data assume a fixed procedure to be performed, selected before the data are examined. In common practice, however, data analysis is an intrinsically adaptive process, with new analyses generated on the basis of data exploration, as well as the results of previous analyses on the same data. We demonstrate a new approach for addressing the challenges of adaptivity based on insights from privacy-preserving data analysis. As an application, we show how to safely reuse a holdout data set many times to validate the results of adaptively chosen analyses.

Reusable holdout method




Any fool
can know.
The point is
to
understand.

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