



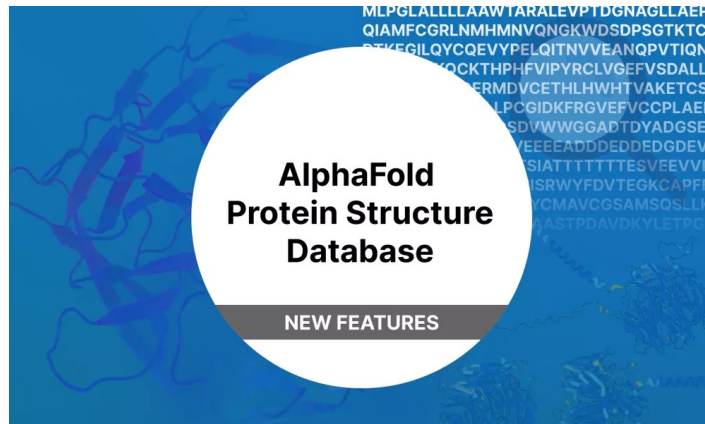
Formalizing AI for science

Indrė Žliobaitė

University of Helsinki

September 22, 2026

Halmstad



nature

Explore content ▾ About the journal ▾ Publish with us ▾

[nature](#) > [articles](#) > [article](#)

Article | [Open access](#) | Published: 15 July 2021

Highly accurate protein structure prediction with AlphaFold

[John Jumper](#) , [Richard Evans](#), [Alexander Pritzel](#), [Tim Green](#), [Michael Figurnov](#), [Olaf Ronneberger](#), [Kathryn Tunyasuvunakool](#), [Russ Bates](#), [Augustin Židek](#), [Anna Potapenko](#), [Alex Bridgland](#), [Clemens Meyer](#), [Simon A. A. Kohl](#), [Andrew J. Ballard](#), [Andrew Cowie](#), [Bernardino Romera-Paredes](#), [Stanislav Nikolov](#), [Rishub Jain](#), [Jonas Adler](#), [Trevor Back](#), [Stig Petersen](#), [David Reiman](#), [Ellen Clancy](#), [Michal Zielinski](#), ... [Demis Hassabis](#) 

[+ Show authors](#)

[Nature](#) **596**, 583–589 (2021) | [Cite this article](#)

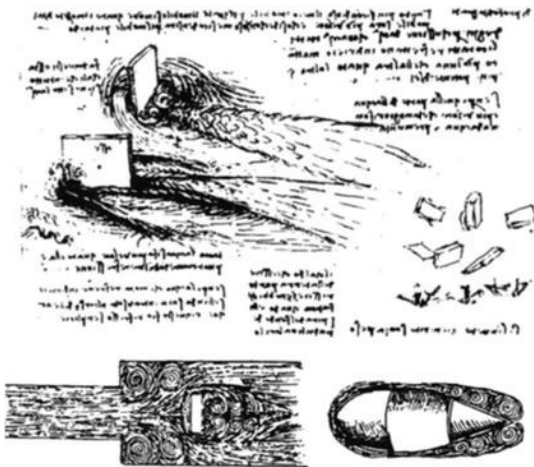
Are these predictions?

Hidden fluid mechanics: Learning velocity and pressure fields from flow visualizations

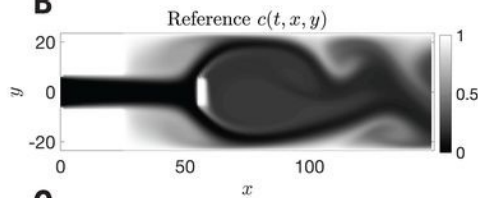
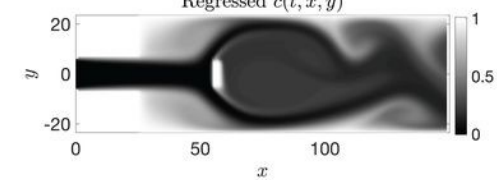
MAZIAR RAISSI  ALIREZA YAZDANI  AND GEORGE EM KARNIADAKIS  [Authors Info & Affiliations](#)

SCIENCE • 30 Jan 2020 • Vol 367, Issue 6481 • pp. 1026-1030 • DOI:10.1126/science.aaw4741

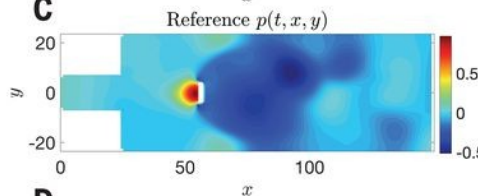
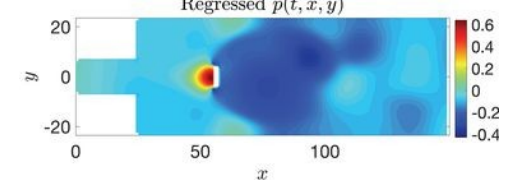
A



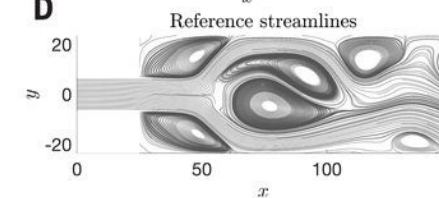
B

Regressed $c(t, x, y)$ 

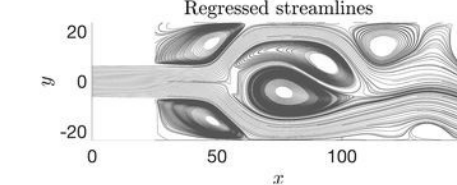
C

Regressed $p(t, x, y)$ 

D



Regressed streamlines



Are these predictions?

AUTOMATION

Description - Classification – Prediction

Evaluation regime:

- Generalization performance
- Robustness
- Agreement with labels

HOME > SCIENCE > VOL. 347, NO. 6226 > CELL TYPES IN THE MOUSE CORTEX AND HIPPOCAMPUS REVEALED BY SINGLE-CELL RNA-SEQ

REPORT



Cell types in the mouse cortex and hippocampus revealed by single-cell RNA-seq

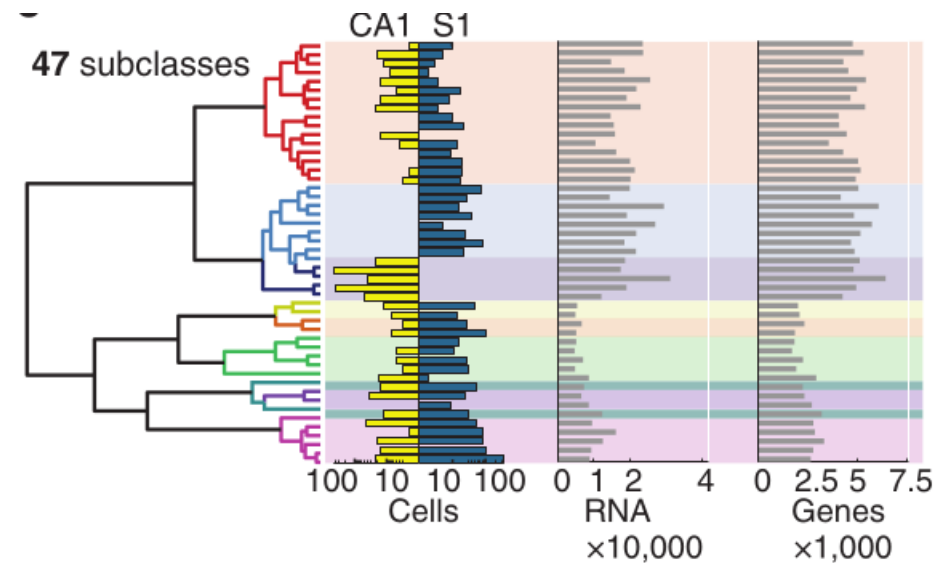
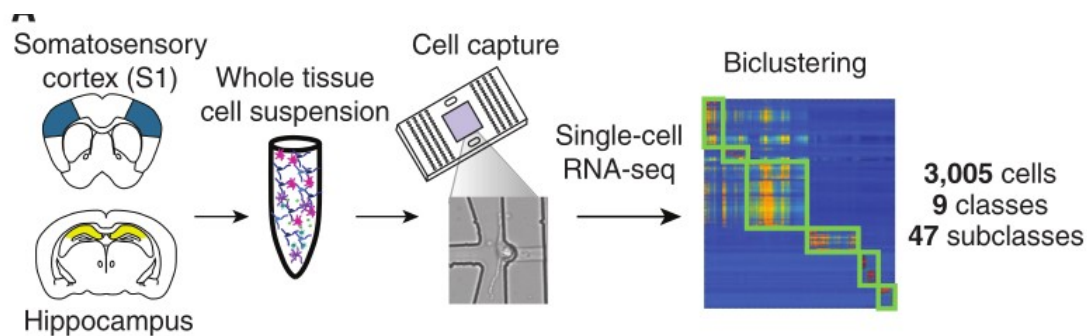
AMIT ZEISEL, ANA B. MUÑOZ-MANCHADO, SIMONE CODELUPPI, PETER LÖNNERBERG, GIOELE LA MANNO, ANNA JURÉUS, SUELI MARQUES, HERMANY MUNGUBA, LIQUN HE, [...]

, AND STEN LINNARSSON

+4 authors

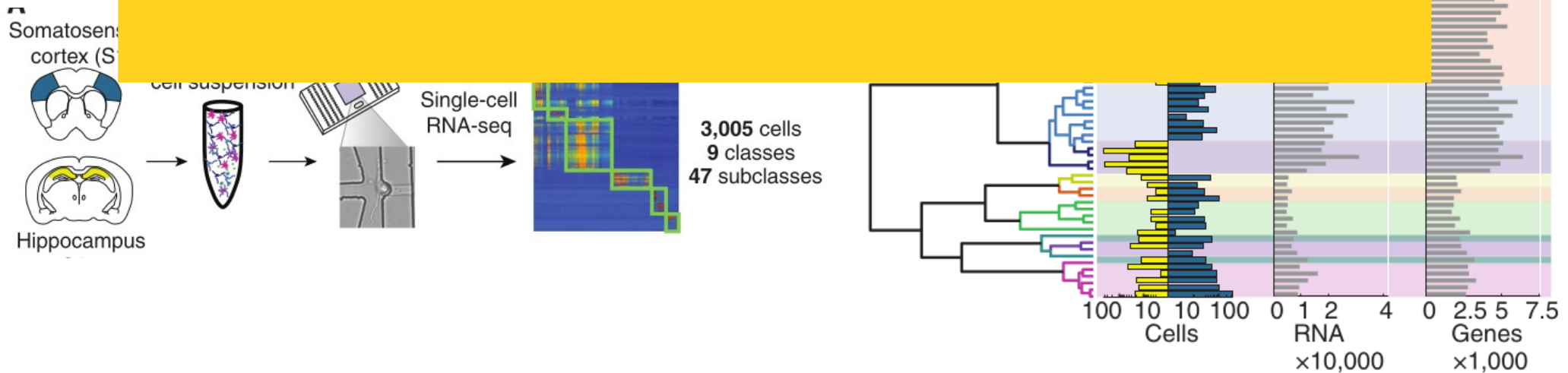
[Authors Info & Affiliations](#)

SCIENCE • 19 Feb 2015 • Vol 347, Issue 6226 • pp. 1138-1142 • DOI: 10.1126/science.aaa1934



Cell types in the mouse cortex and hippocampus re-

claim



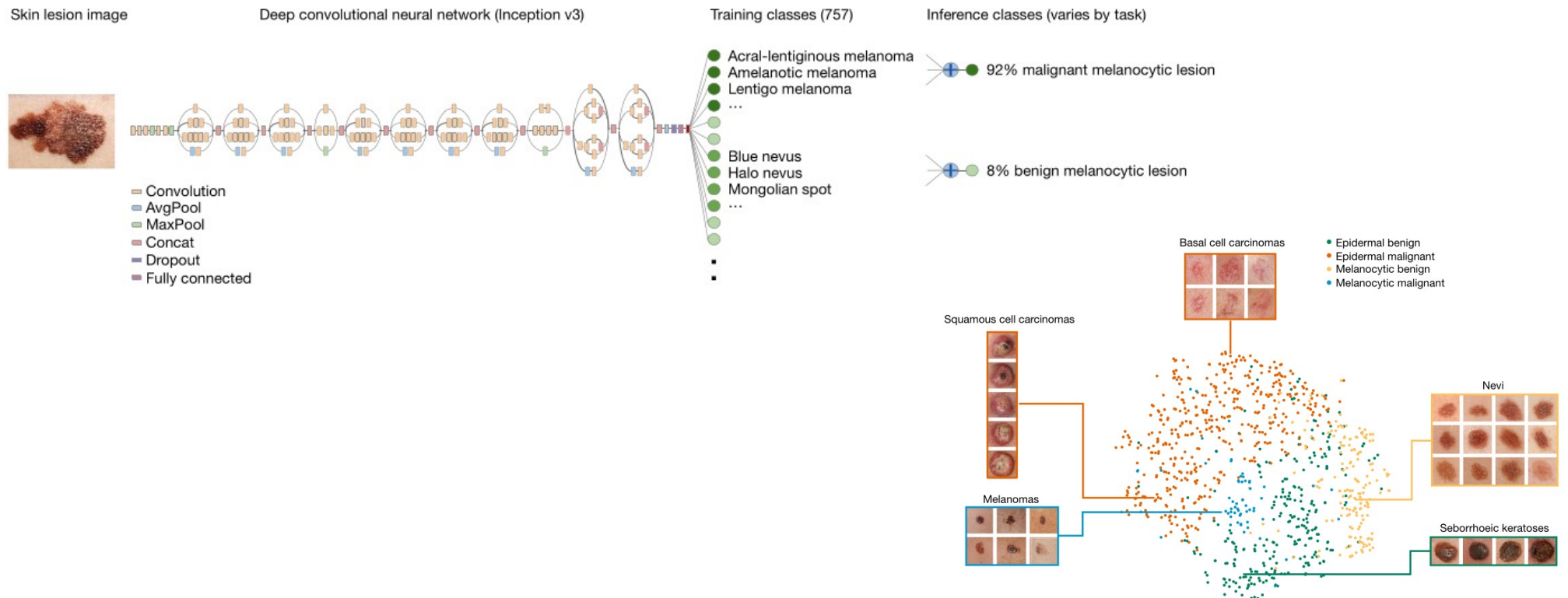
[nature](#) > [letters](#) > article

Letter | Published: 25 January 2017

Dermatologist-level classification of skin cancer with deep neural networks

[Andre Esteva](#) , [Brett Kuprel](#) , [Roberto A. Novoa](#) , [Justin Ko](#), [Susan M. Swetter](#), [Helen M. Blau](#) & [Sebastian Thrun](#) 

[Nature](#) **542**, 115–118 (2017) | [Cite this article](#)



[nature](#) > [letters](#) > article

Letter | Published: 25 January 2017

Dermatologist-level classification of skin cancer with deep neural networks

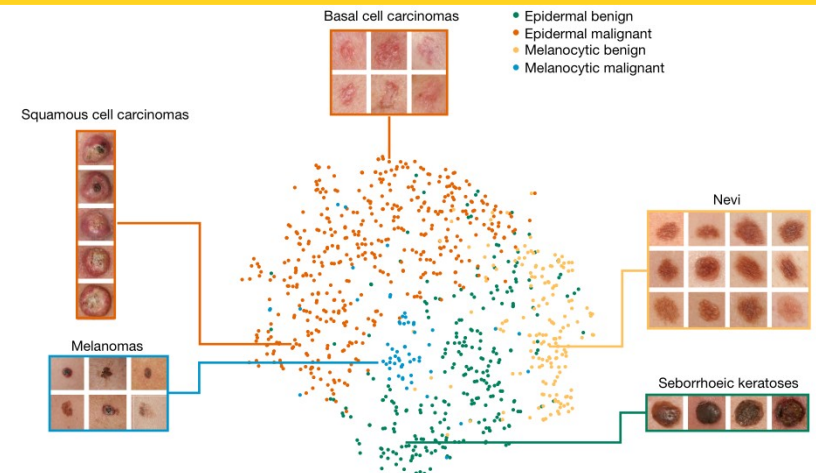
M c claim

Skin lesion image



■ Concat
 ■ Dropout
 ■ Fully connected

■
 ■
 ■



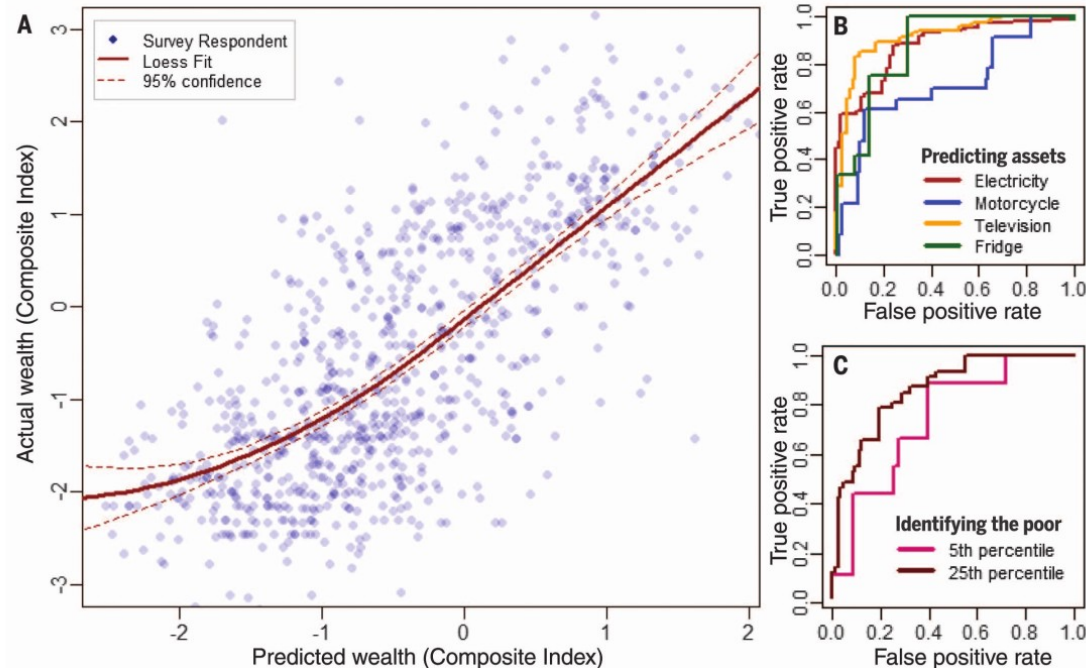
REPORT



Predicting poverty and wealth from mobile phone metadata

JOSHUA BLUMENSTOCK, GABRIEL CADAMURO, AND ROBERT ON [Authors Info & Affiliations](#)

SCIENCE • 27 Nov 2015 • Vol 350, Issue 6264 • pp. 1073-1076 • DOI: 10.1126/science.aac4420

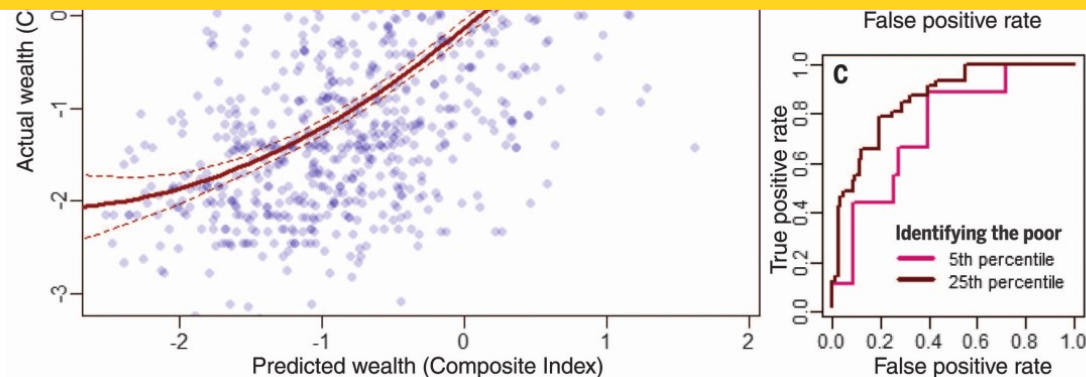


🔒 | REPORT



Predicting poverty and wealth from mobile phone

G claim



SCIENTIFIC THEORY CONSTRUCTION

Evaluation regime:

- Explanatory coherence
- Interventional stability

AUTOMATION

Description - Classification – Prediction

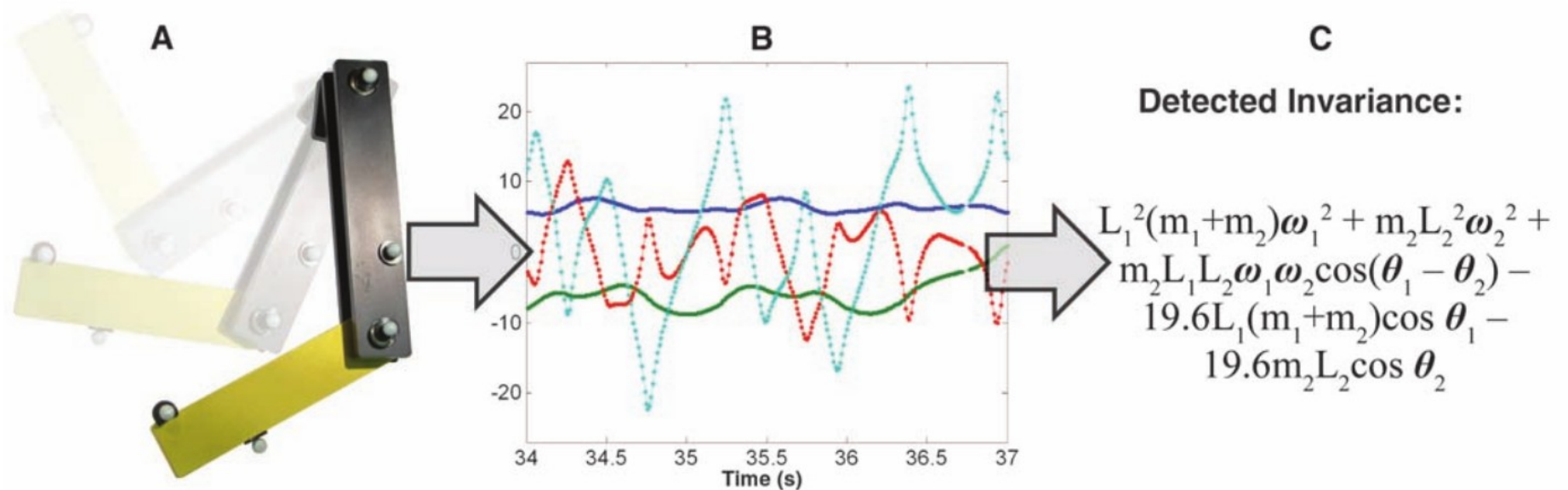
Evaluation regime:

- Generalization performance
- Robustness
- Agreement with labels

*Standard ML
evaluation
largely
sufficient*

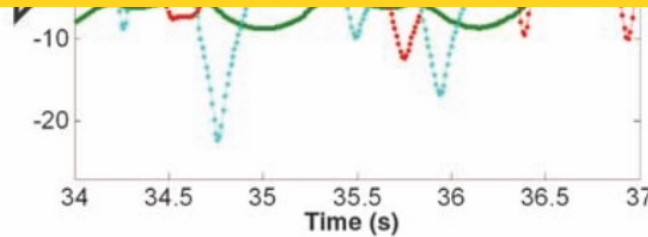
Distilling Free-Form Natural Laws from Experimental Data

MICHAEL SCHMIDT AND HOD LIPSON [Authors Info & Affiliations](#)



Distilling Free-Form Natural Laws from Experimental

T claim



$$19.6L_1(m_1+m_2)\cos\theta_1 - 19.6m_2L_2\cos\theta_2$$

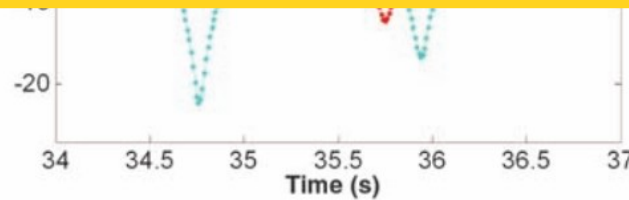
Distilling Free-Form Natural Laws from Experimental Data

MICHAEL SCHMIDT AND HOD LIPSON [Authors Info & Affiliations](#)

A**B****C**

≠ causality

variance:



$$\begin{aligned} &+ m_2 L_2^2 \omega_2^2 + \\ &\cos(\theta_1 - \theta_2) - \\ &m_2) \cos \theta_1 - \\ &19.6 m_2 L_2 \cos \theta_2 \end{aligned}$$

SCIENTIFIC THEORY CONSTRUCTION

Evaluation regime:

- Explanatory coherence
- Interventional stability

*Hybrid
human-
machine
reasoning*

AUTOMATION

Description - Classification – Prediction

Evaluation regime:

- Generalization performance
- Robustness
- Agreement with labels

*Standard ML
evaluation
largely
sufficient*

SCIENTIFIC THEORY CONSTRUCTION

Evaluation regime:

- Explanatory coherence
- Interventional stability

*Hybrid
human-
machine
reasoning*

MEASUREMENT

Evaluation regime:

- Stability across retraining
- Calibration to reference standards
- Cross-context comparability

*Predictive
accuracy
alone
insufficient*

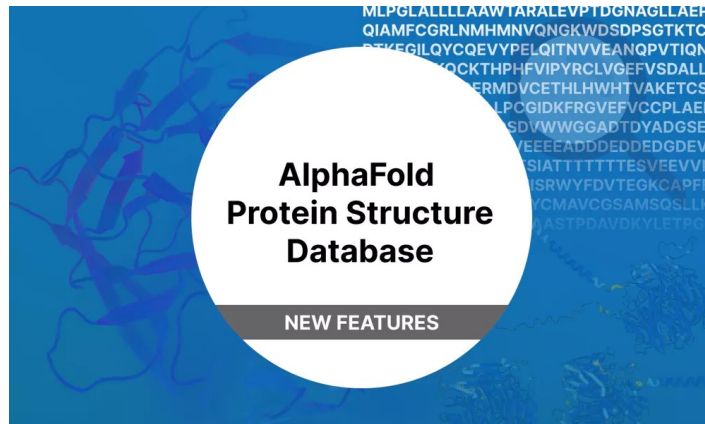
AUTOMATION

Description - Classification – Prediction

Evaluation regime:

- Generalization performance
- Robustness
- Agreement with labels

*Standard ML
evaluation
largely
sufficient*



nature

Explore content ▾ About the journal ▾ Publish with us ▾

[nature](#) > [articles](#) > [article](#)

Article | [Open access](#) | Published: 15 July 2021

Highly accurate protein structure prediction with AlphaFold

[John Jumper](#) , [Richard Evans](#), [Alexander Pritzel](#), [Tim Green](#), [Michael Figurnov](#), [Olaf Ronneberger](#), [Kathryn Tunyasuvunakool](#), [Russ Bates](#), [Augustin Židek](#), [Anna Potapenko](#), [Alex Bridgland](#), [Clemens Meyer](#), [Simon A. A. Kohl](#), [Andrew J. Ballard](#), [Andrew Cowie](#), [Bernardino Romera-Paredes](#), [Stanislav Nikolov](#), [Rishub Jain](#), [Jonas Adler](#), [Trevor Back](#), [Stig Petersen](#), [David Reiman](#), [Ellen Clancy](#), [Michal Zielinski](#), ... [Demis Hassabis](#) 

[+ Show authors](#)

[Nature](#) **596**, 583–589 (2021) | [Cite this article](#)

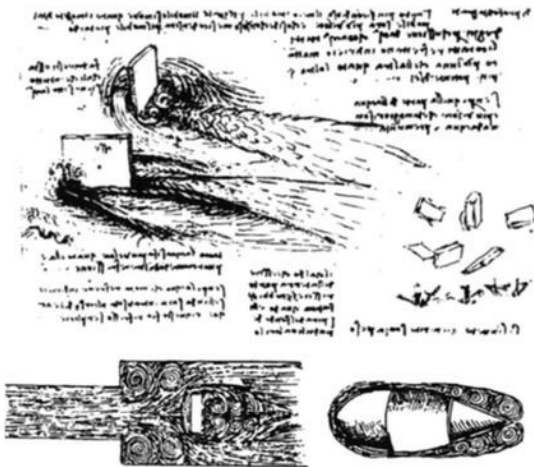
Stabilized measurement

Hidden fluid mechanics: Learning velocity and pressure fields from flow visualizations

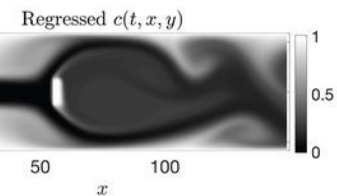
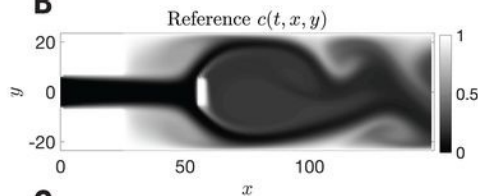
MAZIAR RAISSI  ALIREZA YAZDANI  AND GEORGE EM KARNIADAKIS  [Authors Info & Affiliations](#)

SCIENCE • 30 Jan 2020 • Vol 367, Issue 6481 • pp. 1026-1030 • DOI:10.1126/science.aaw4741

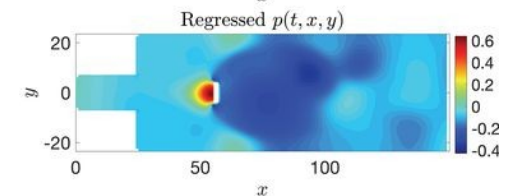
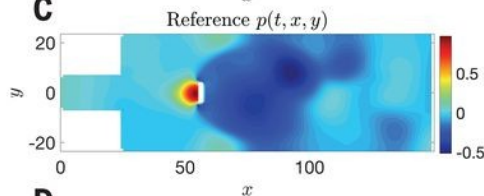
A



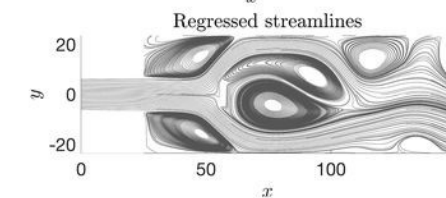
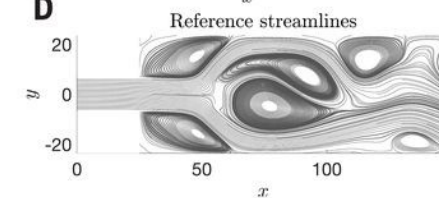
B



C



D



Provisional measurement



SCIENTIFIC THEORY CONSTRUCTION

Evaluation regime:

- Explanatory coherence
- Interventional stability

*Hybrid
human-
machine
reasoning*

MEASUREMENT

Provisional and Stabilized measurement

Evaluation regime:

- Stability across retraining
- Calibration to reference standards
- Cross-context comparability

*Predictive
accuracy
alone
insufficient*

AUTOMATION

Description - Classification – Prediction

Evaluation regime:

- Generalization performance
- Robustness
- Agreement with labels

*Standard ML
evaluation
largely
sufficient*

MEASUREMENT

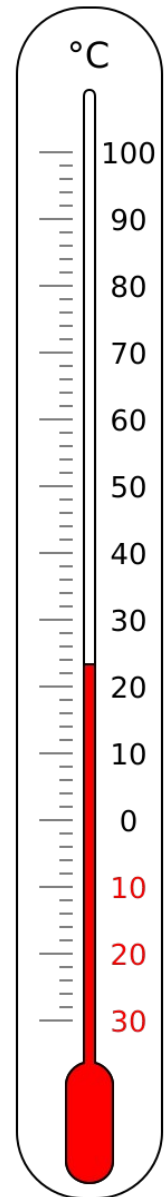
Provisional and Stabilized measurement

Evaluation regime:

- | | |
|--------------------------------------|---------------------|
| • Stability across retraining | <i>Predictive</i> |
| • Calibration to reference standards | <i>accuracy</i> |
| • Cross-context comparability | <i>alone</i> |
| | <i>insufficient</i> |

When measurement instruments learn

- Classical instruments
 - Fixed physically motivated mappings
 - Separation of measurement vs. inference/interpretation
 - Human-centered epistemic responsibility
- Learned (AI-based) instruments
 - Non-unique calibration (model fitting)
 - Measurement and inference often inseparable
 - Delegation of responsibility



[Home](#) / [Uncategorized](#) / [AI Thermometer](#)

AI Thermometer

\$69.99

In stock

1 ▾

Add to cart

SKU: SMK3 Categories: [AI Thermometers](#), [Covid Testing](#), [Uncategorized](#)



HIGH TEMPERATURE ALARM

Complete Alarm Of Temperature Anomaly 10

TO NEVER REPEAT

Temperature Anomaly 10

W

Intuition

- We need stability across admissible realizations
- What is an admissible realization?
 - Reasonable parameter settings
 - Reasonable accuracy
 - Variants that ML practitioners would reasonably consider

Formalizing learned measurement functions

- Standard supervised learning
 - Accuracy (gen.), calibration, robustness

Formalizing learned measurement functions

- Standard supervised learning
 - Accuracy (gen.), calibration, robustness
- Measurement stability

$$m_1(o_1, c_1 | z) \approx m_2(o_2, c_2 | z),$$

m model, o observations, c contexts, z ground truth target

Formalizing learned measurement functions

- Standard supervised learning
 - Accuracy (gen.), calibration, robustness
- Measurement stability

$$m_1(o_1, c_1 | z) \approx m_2(o_2, c_2 | z),$$

m model, o observations, c contexts, z ground truth target

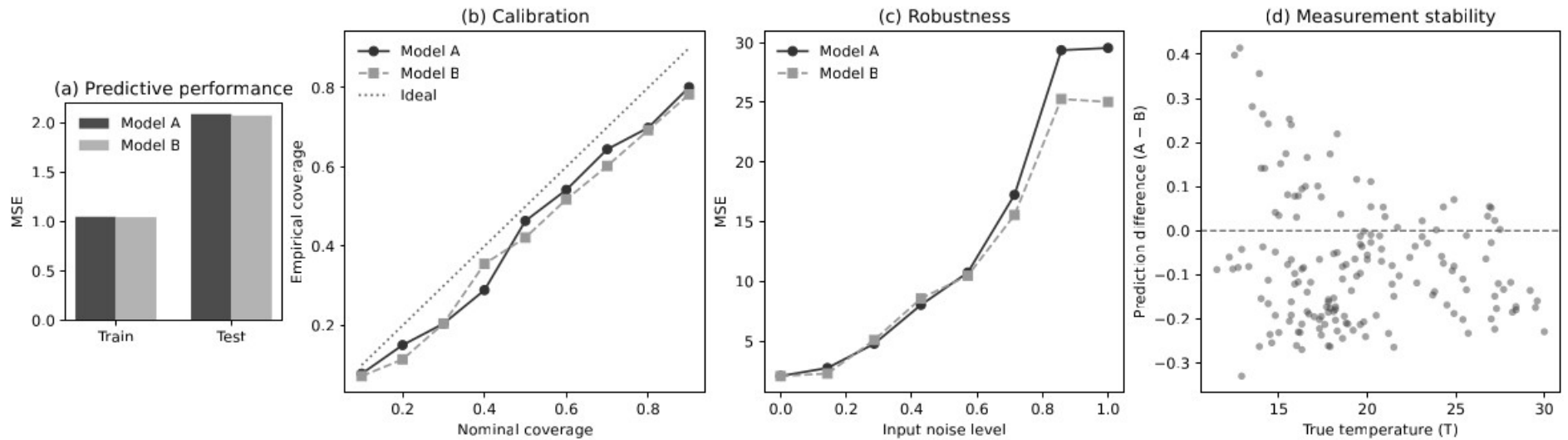
- Robustness

$$m(o) \approx m(o + d),$$

d perturbation/noise

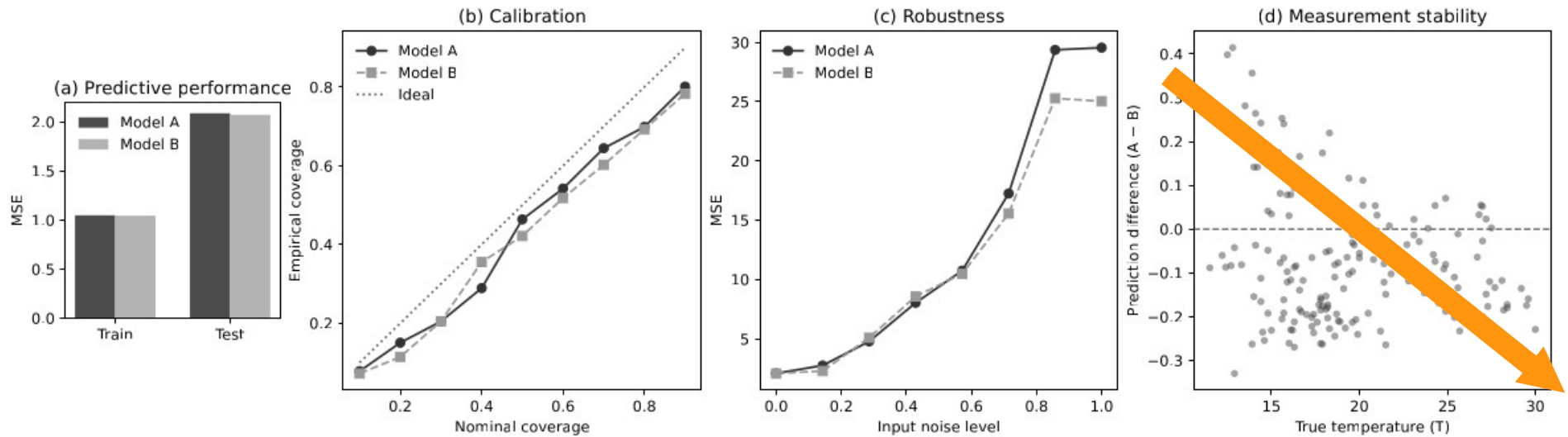
Empirical evidence

UCI Air Quality Dataset



Regression, different feature subsets

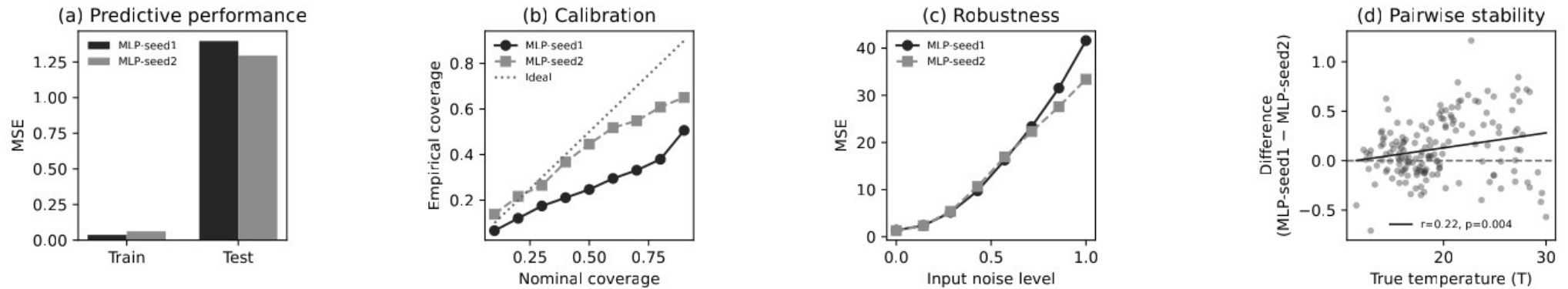
Empirical evidence



Neither of the models
implement
measurement

Empirical evidence

Stable as a
measurement

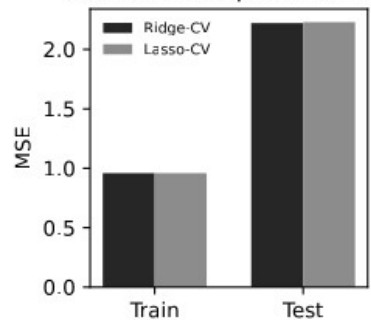


MLP, different random seeds

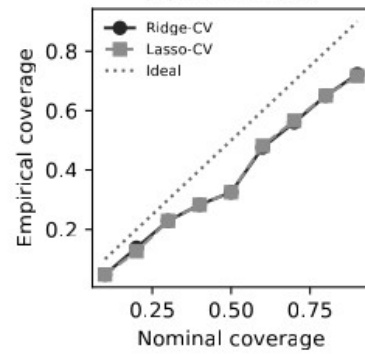
Empirical evidence

Very unstable,
systematic bias

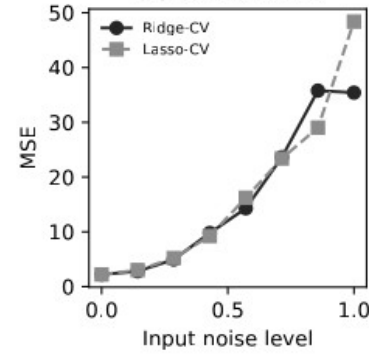
(a) Predictive performance



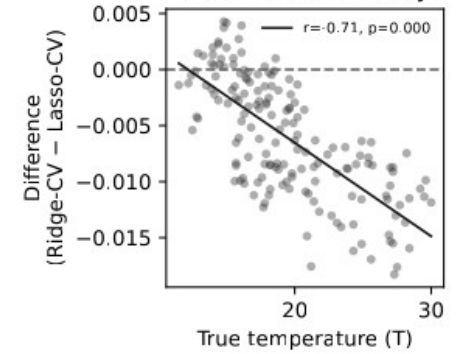
(b) Calibration



(c) Robustness



(d) Pairwise stability



Regression, different regularization

Implications for modelling

- The evaluative question shifts
 - from “**Does this predict well?**”
 - to “**Do admissible realisations agree on what is being measured?**”
- Accuracy, calibration and robustness are necessary but not sufficient
- Measurement stability is relative

Challenges

- Which realizations are admissible?
- Which models are independent?
- Consensus ensemble?

Epistemic risks and responsibilities

- Users do not know modeling assumptions
- Tool makers and users may have misaligned incentives and expertise
 - Especially in interdisciplinary settings
- Lack of portability/reproducibility across labs
- Who is responsible for the conclusions?

Daily briefing: Machine learning discovers antibiotics

AI helps to fight resistant bacteria, China to clamp down on wildlife trade and warm water spied under Antarctic glacier

By [Emma Stoye](#)



Sign up for Nature Briefing

Hello *Nature* readers, would you like to get this Briefing in your inbox free every day? [Sign up here](#)



Escherichia coli bacteria, coloured green, in a scanning electron micrograph. Credit: Stephanie Schuller/SPL

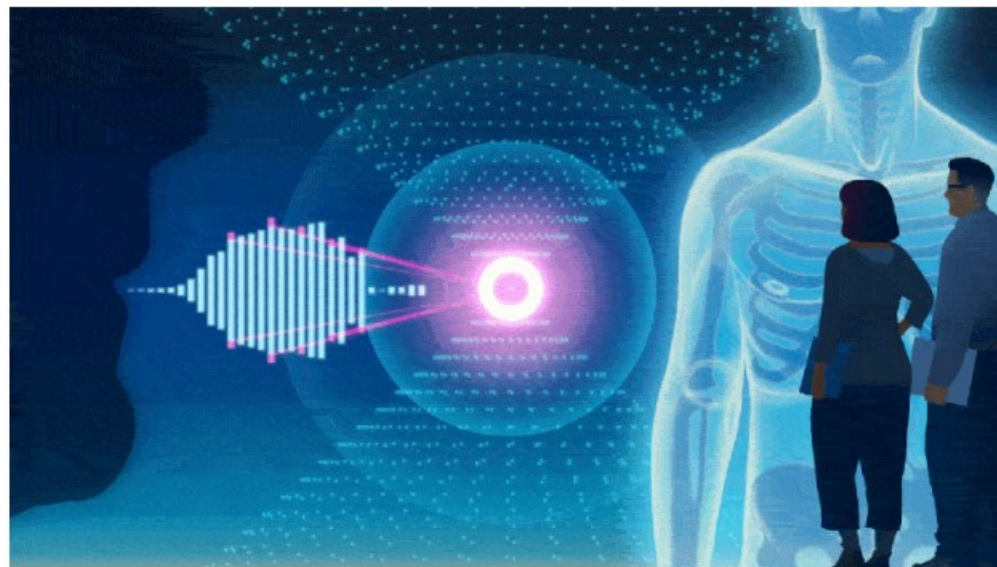
[nature](#) > [outlook](#) > article

OUTLOOK | 22 May 2025

AI listens for health conditions

Voice recordings, examined by artificial intelligence, might provide new biomarkers for conditions such as heart disease and Alzheimer's.

By [Neil Savage](#)



Credit: Sam Chivers

[nature](#) > [nature reviews bioengineering](#) > [editorials](#) > [article](#)

Editorial | Published: 15 January 2026

AI challenges science to reinvent itself

[Nature Reviews Bioengineering](#) 4, 1 (2026) | [Cite this article](#)

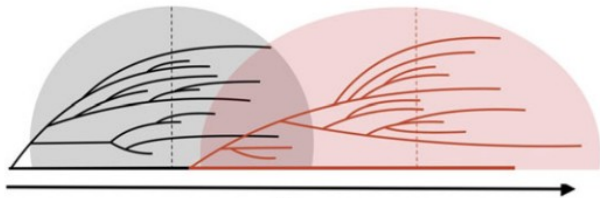
2813 Accesses | 2 Altmetric | [Metrics](#)

As artificial intelligence enters the scientific arena, it not only compels us to rethink the scientific method but also opens the door to reimagine long-standing practices.

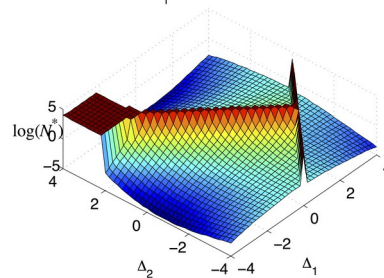
Group leader: Indrė Žliobaitė, Professor
indre.zliobaite@helsinki.fi

DATA SCIENCE AND EVOLUTION GROUP

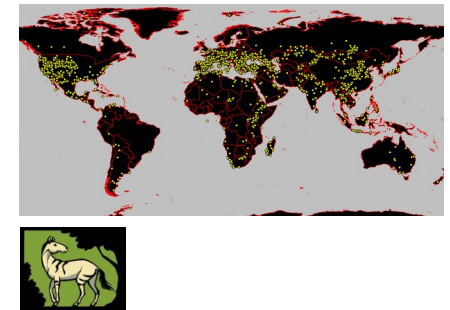
Complex systems
change processes
in nature and society



Computational methods
for science,
special focus on evolving data



**Scientific data and
open science**



Teaching focus:
Trustworthy ML
Interdisciplinary data science

Main collaborating institutions



Research funding

