Prediction and it limits for scientific discovery

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pervasive desire to predict science

- **what will be discovered?** 🔮
- **by whom, when, and where?**

pervasive desire to predict science

- **what will be discovered?**
- **by whom, when, and where?**

individuals	what questions are useful, impactful, fundable?
publishers, funders	what manuscripts or projects will be most impactful?
hiring committees	which applicant will perform best? which will make most valuable contributions?
society	how can tax and other dollars be invested to make technological, biomedical, and scientific advances?

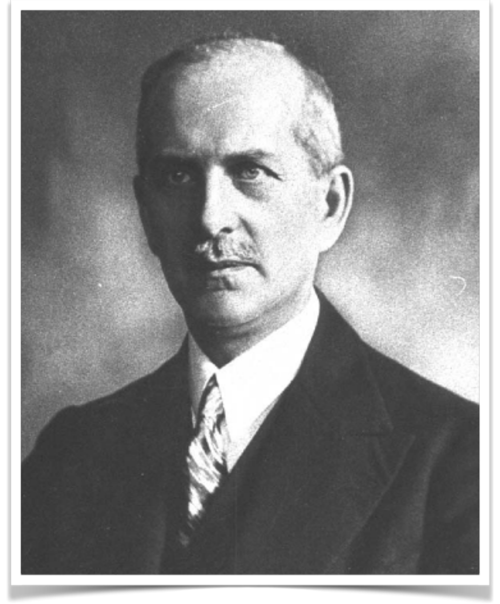
how *predictable* are scientific discoveries?

- **simple question with a 150+ year history**

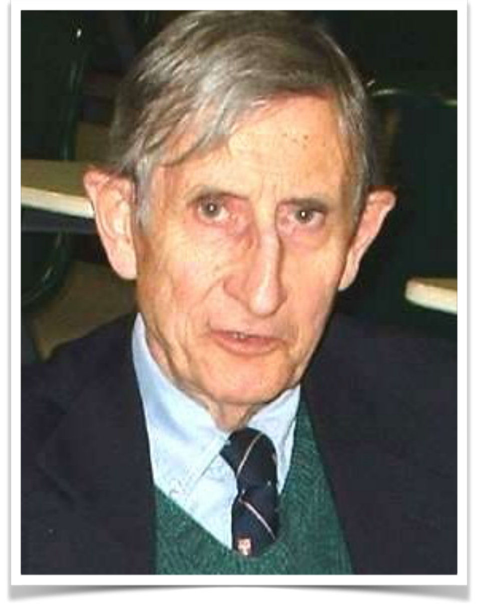
how *predictable* are scientific discoveries?

- **simple question with a 150+ year history**

Bolesław Prus
(1847-1912)



Florian Znaniecki
(1882-1958)



Freeman Dyson
(1923-2020)

Steven Weinberg
(1933-)

Harriet Zuckerman
(1937-)

. . .

- philosophy, physics, sociology…
- mainly conceptual, focusing on goals and general approaches
  (Weinberg: "to explain the world") (Dyson: "birds and frogs")
- progress toward a genuine "science of science" was slow
  - hard to get good data
  - judgement of experts seemed good enough

* this question complements the old and rich literature on the sociology of science: who gets to make discoveries?

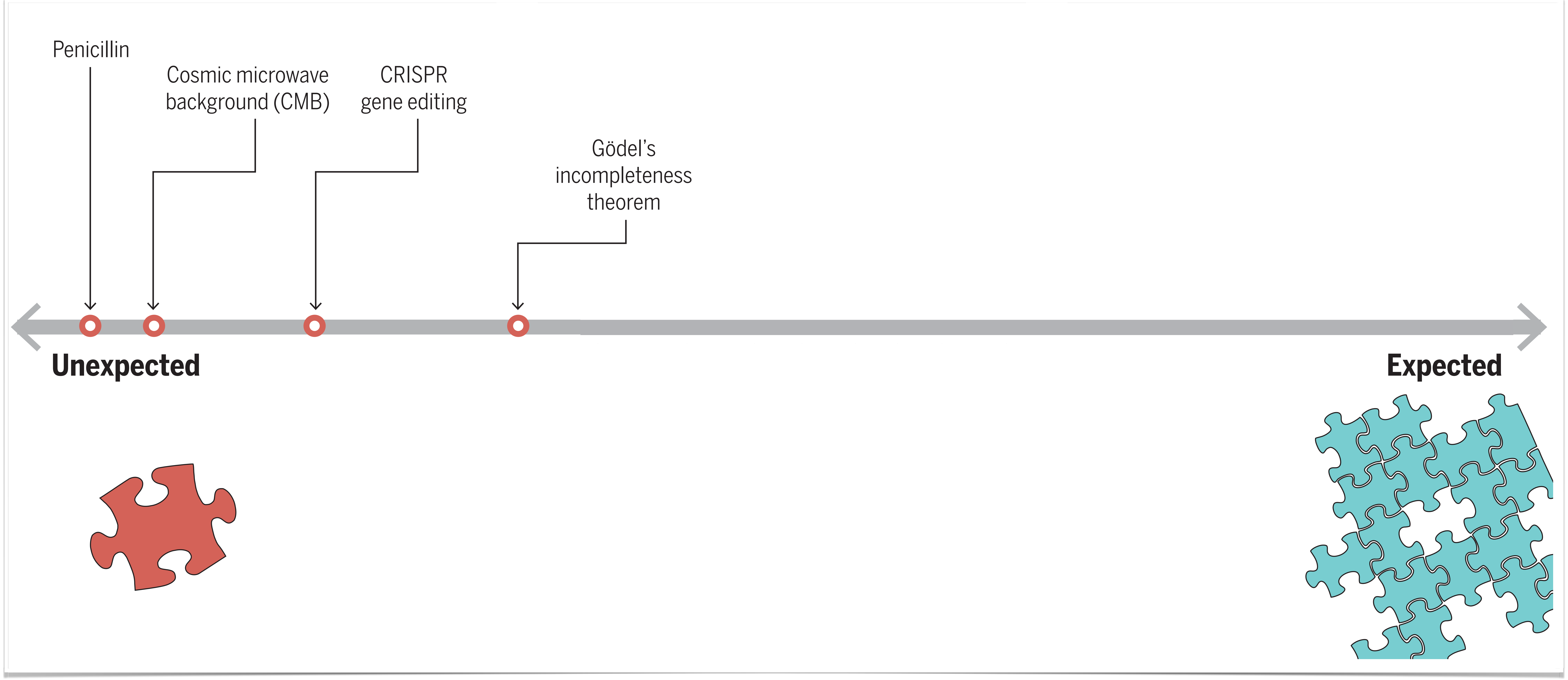
predictability depends on context

Clauset, Larremore & Sinatra, Science 355, 477-480 (2017)

predictability depends on context

unexpected discovery

changes the way we understand the world, or finds novel use elsewhere

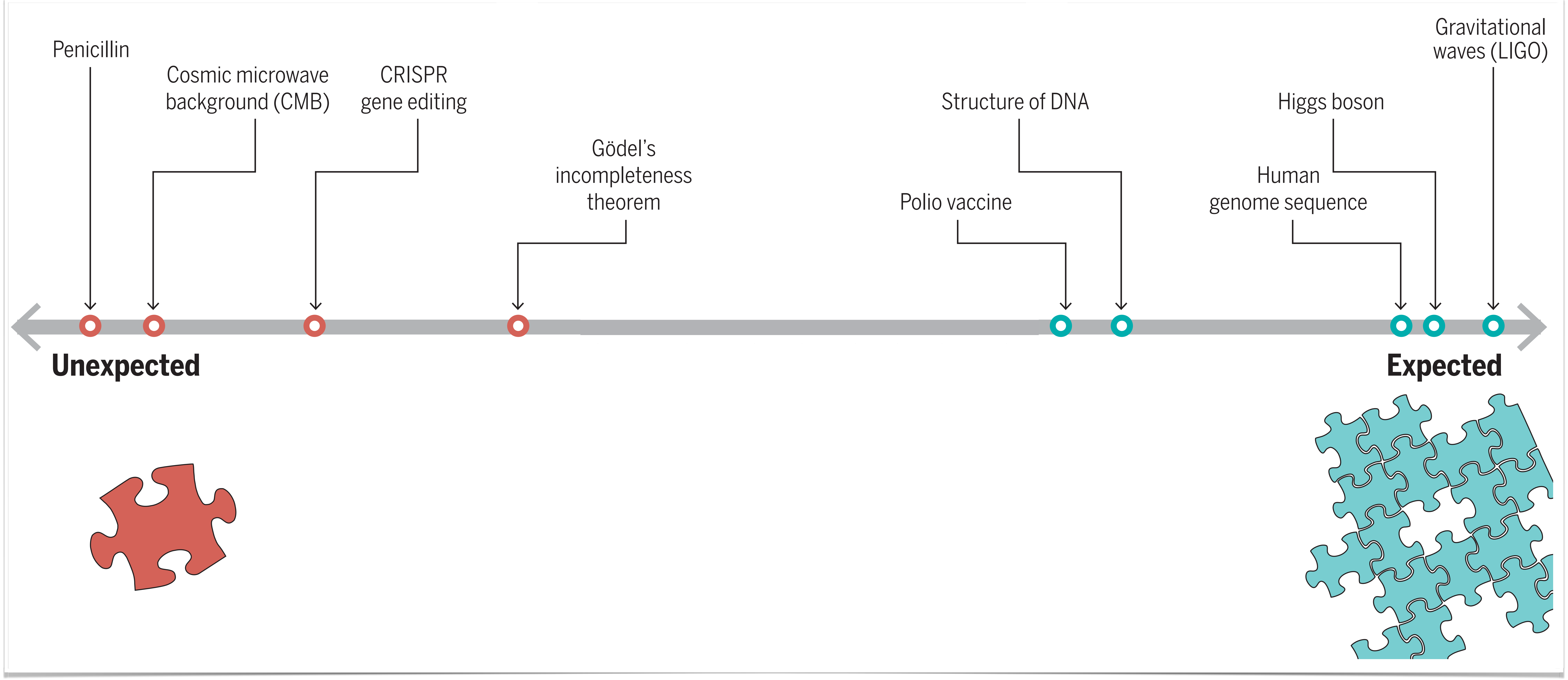


Clauset, Larremore & Sinatra, Science 355, 477-480 (2017)

predictability depends on context

expected discovery

accumulation of theory and evidence, fits with other ideas

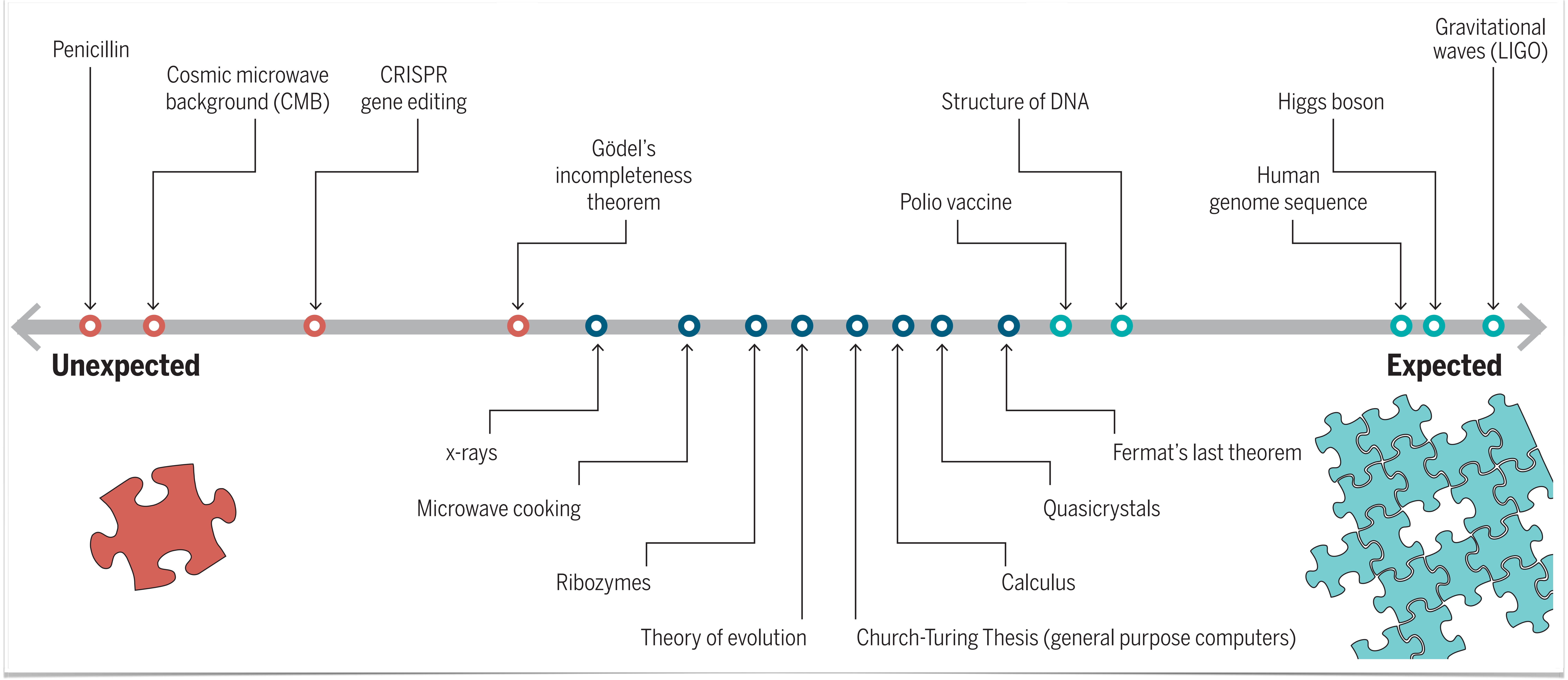


Clauset, Larremore & Sinatra, Science 355, 477-480 (2017)

predictability depends on context

"normal" discovery

some elements surprising, but fits partly within existing ideas



Clauset, Larremore & Sinatra, Science 355, 477-480 (2017)

a modern science of science

predicting discovery

a modern science of science

predicting discovery

- abundant data
  - (1) publications + citation networks, (2) people, (3) funding
  - Google Scholar, PubMed, Web of Science, arXiv, JSTOR, OCRID, EasyChair, NIH, NSF, patents, CVs, etc.
- abundant computation
- growing interdisciplinary community
  - computer scientists, information scientists, economists, sociologists, statisticians, physicists, biologists, etc.

surely all this data must enable better predictions of future discoveries!

a modern science of science

predicting discovery

- **surely all this data must enable better predictions of future discoveries?**

APS Data Sets for Research

WEB OF SCIENCE™

JSTOR

dblp
computer science bibliography

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PubMed

a modern science of science

predicting discovery

- **surely all this data must enable better predictions of future discoveries?**
- yes, but…

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a modern science of science

predicting discovery

- **surely all this data must enable better predictions of future discoveries?**
- yes, but…
  - the data are crude + biased + noisy + incomplete : *they don't directly measure knowledge or progress*
  - what things *are* predictable and what things *are not*?

productivity over a career

the canonical narrative (50+ years of evidence):

- **rapid rise to an early peak**
- **decline or flattening**

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publication rates in psychology, 1986 ✓

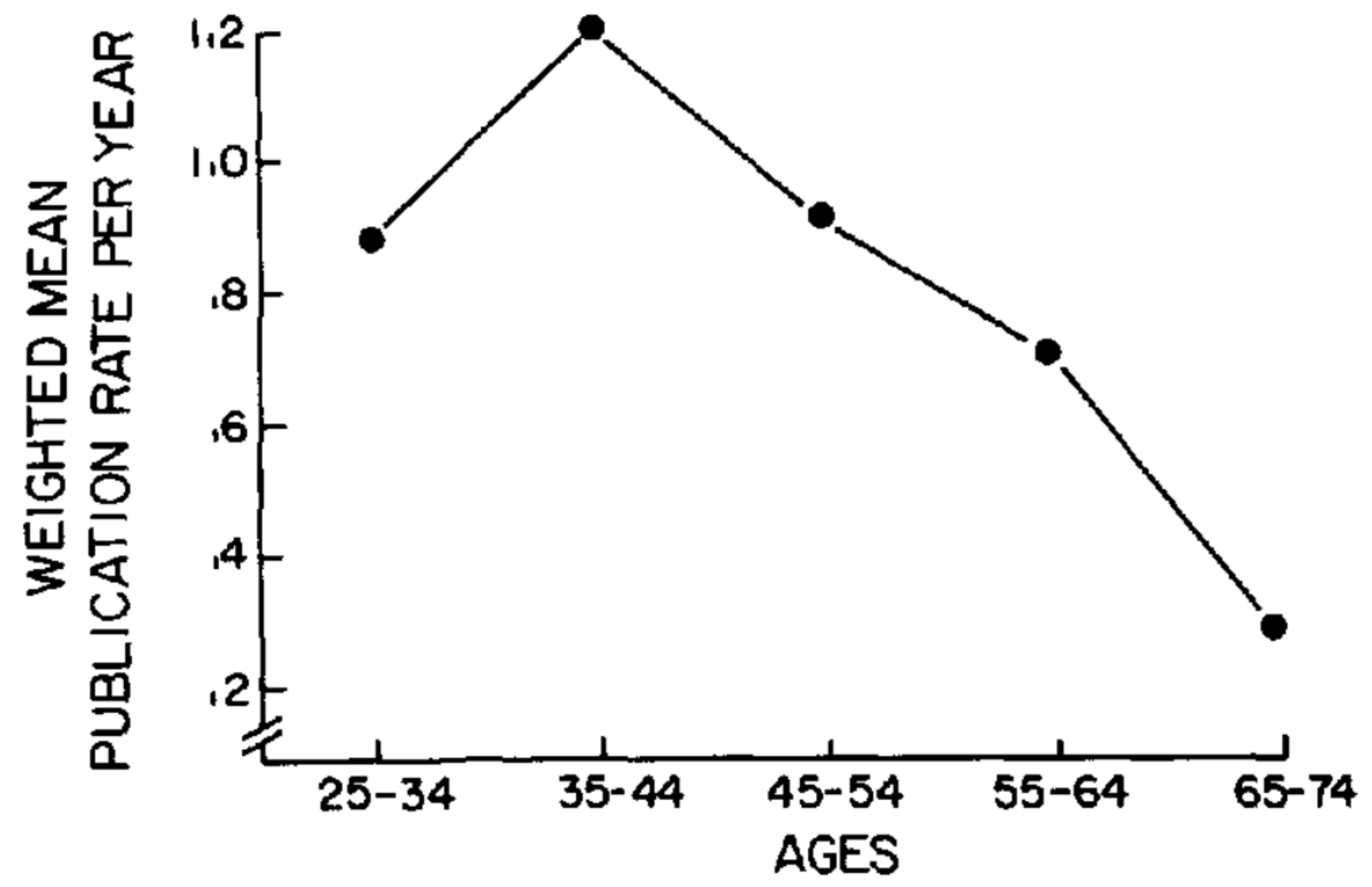

Figure 1. Weighted mean publication rate per year for 1,084 North American academic psychologists at five age intervals.

Horner, et al. Psychology and Aging 1(4), 319 (1986)

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publication rates in psychology, 1986 ✓

. . . in Russian science & math, 1954 ✓

FIG. 1. Age versus creative production rate for Russians only, in science and mathematics.

Lehman, The Scientific Monthly 78, 321-326 (1954)

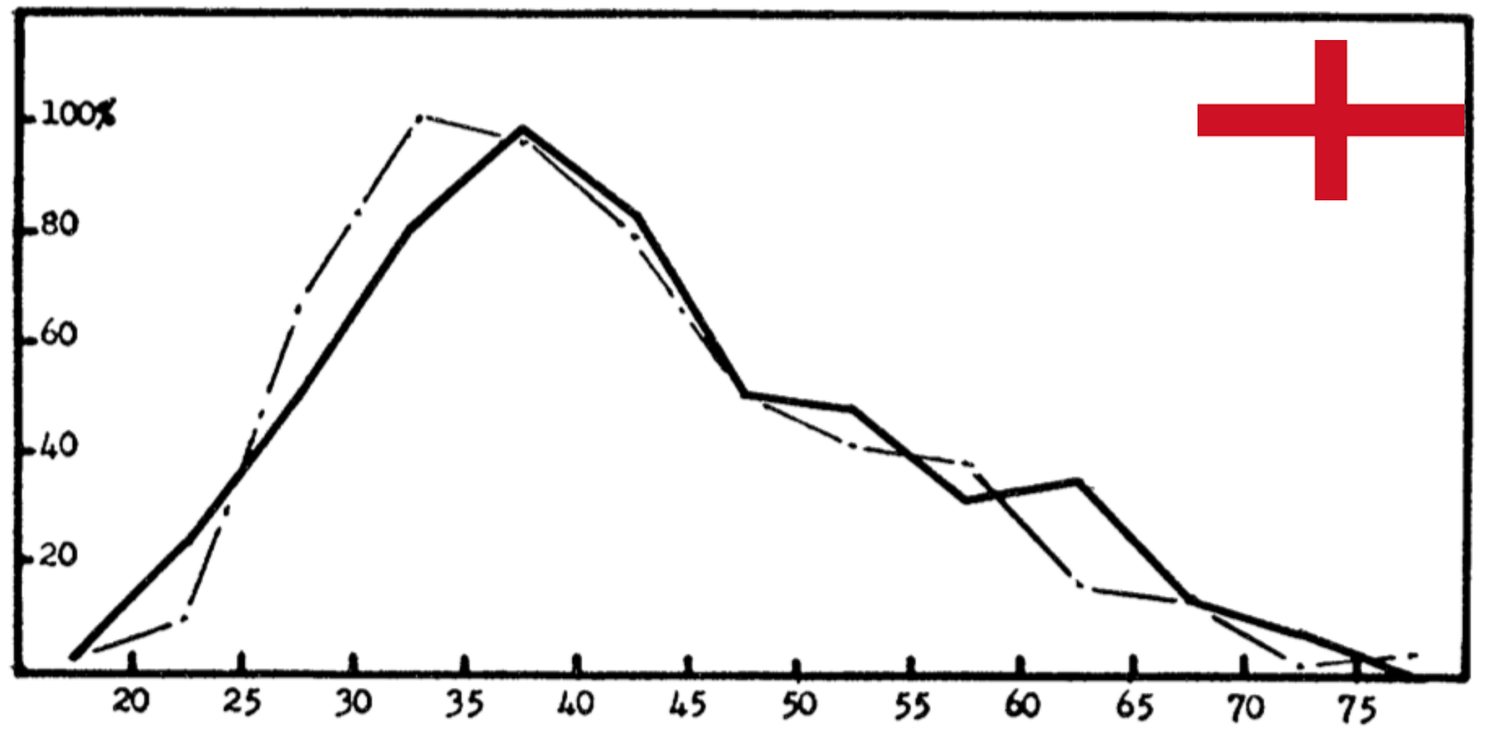

FIG. 2. Solid line: age versus creative production rate for Englishmen only, in science and mathematics. Broken line, same as Fig. 1.

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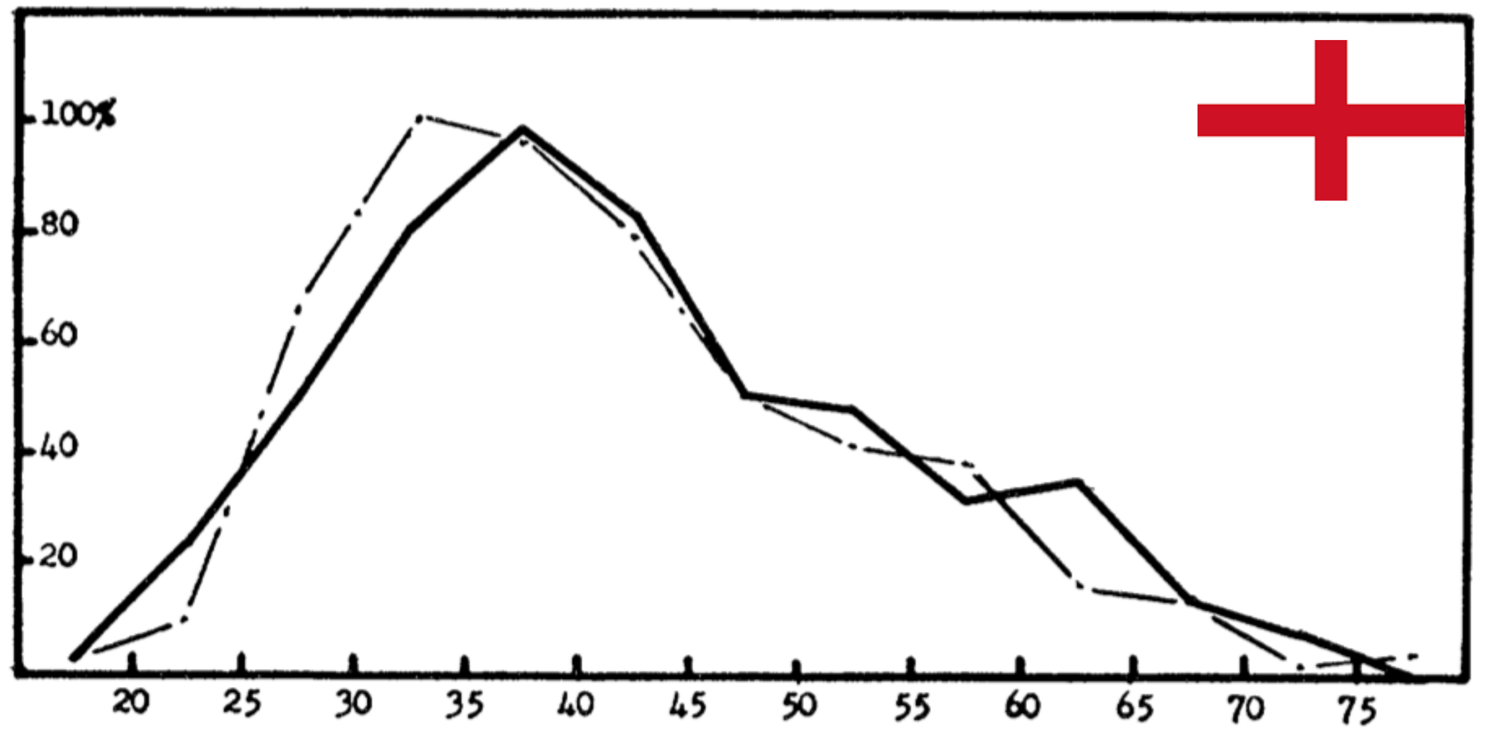

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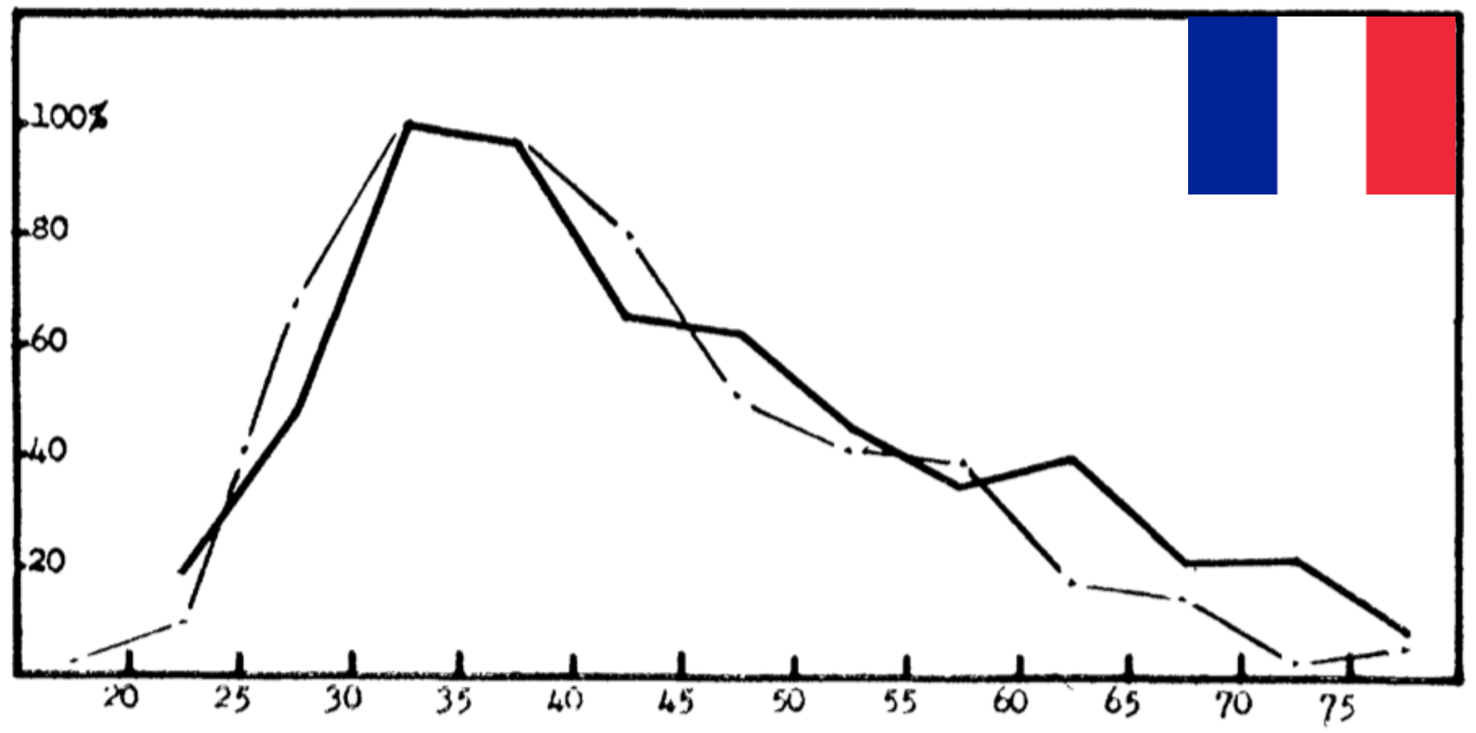

FIG. 3. Solid line: age versus creative production rate for Frenchmen only, in science and mathematics. Broken line, same as Fig. 1.

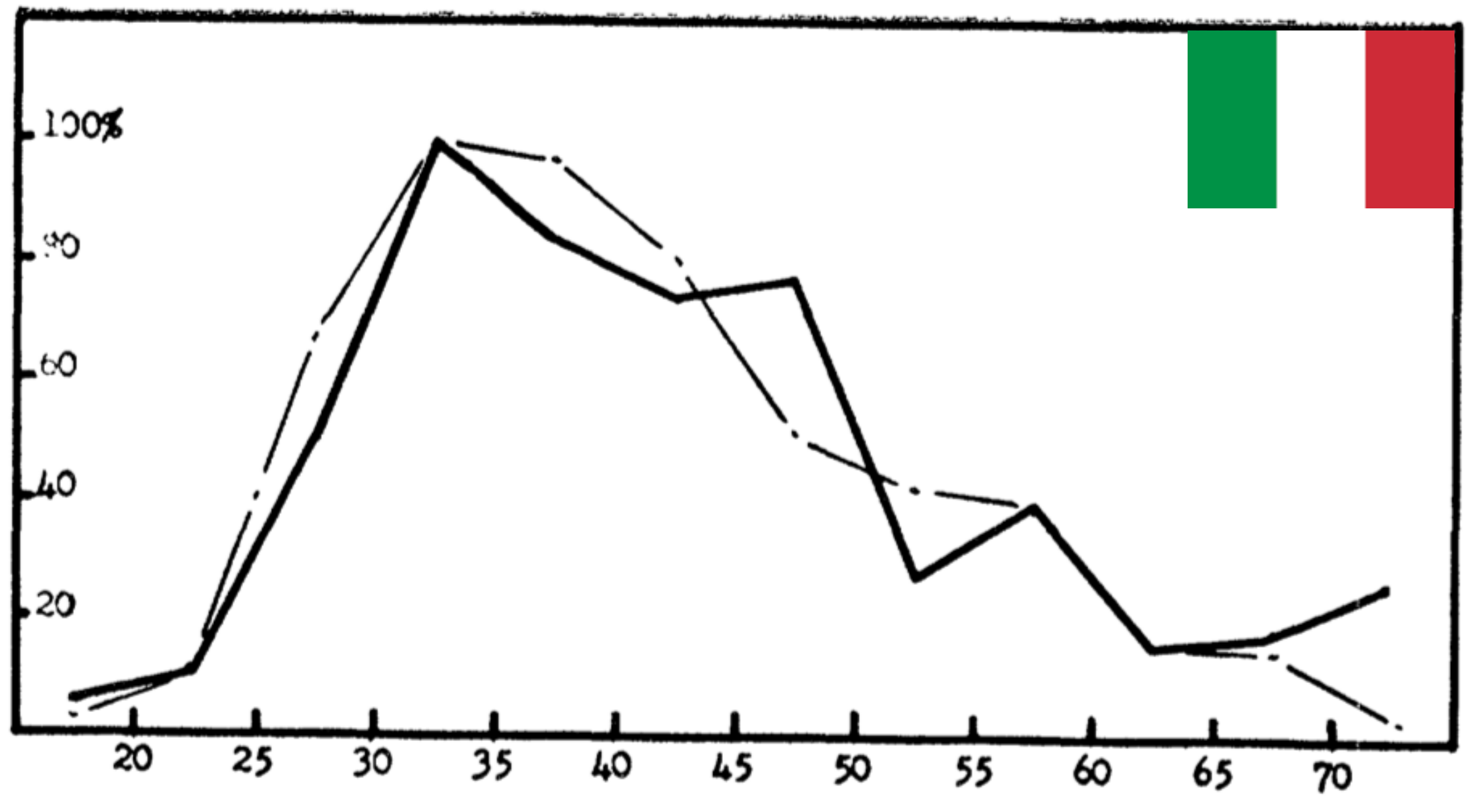

FIG. 4. Solid line: age versus creative production rate for Italians only, in science and mathematics. Broken line, same as Fig. 1.

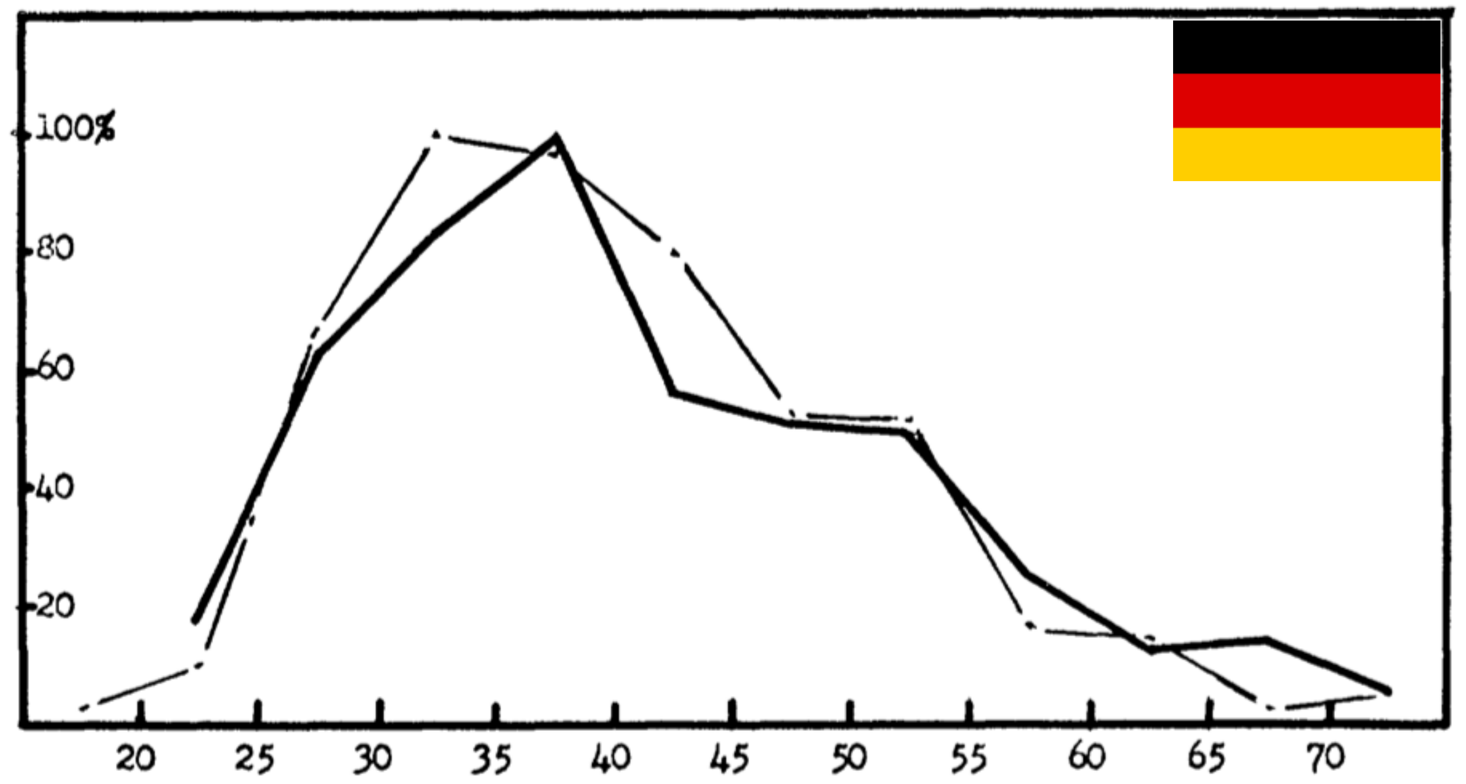

FIG. 5. Solid line: age versus creative production rate for Germans only, in science and mathematics. Broken line, same as Fig. 1.

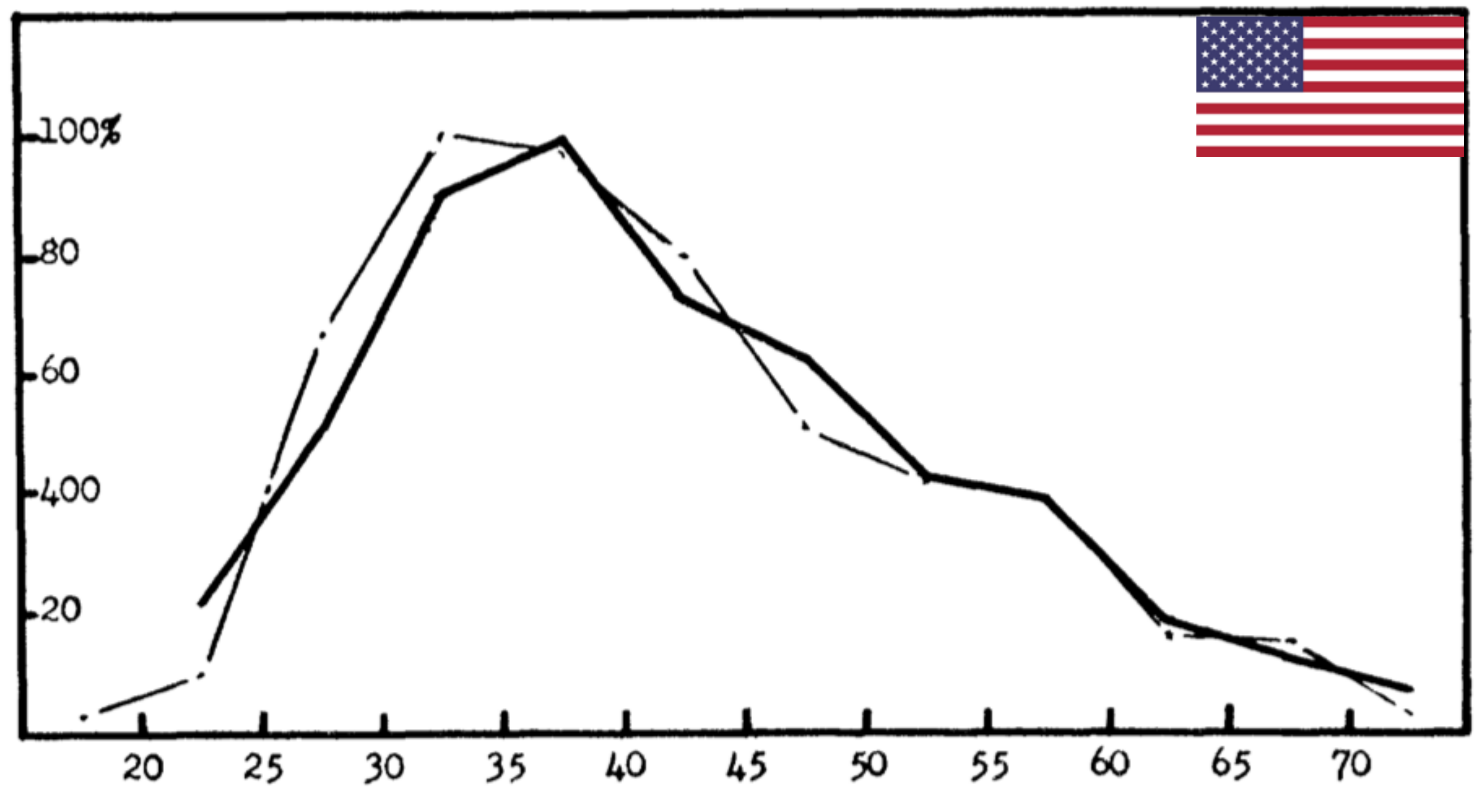

FIG. 6. Solid line: age versus creative production rate for individuals from the U.S.A. only, in science and mathematics. Broken line, same as Fig. 1.

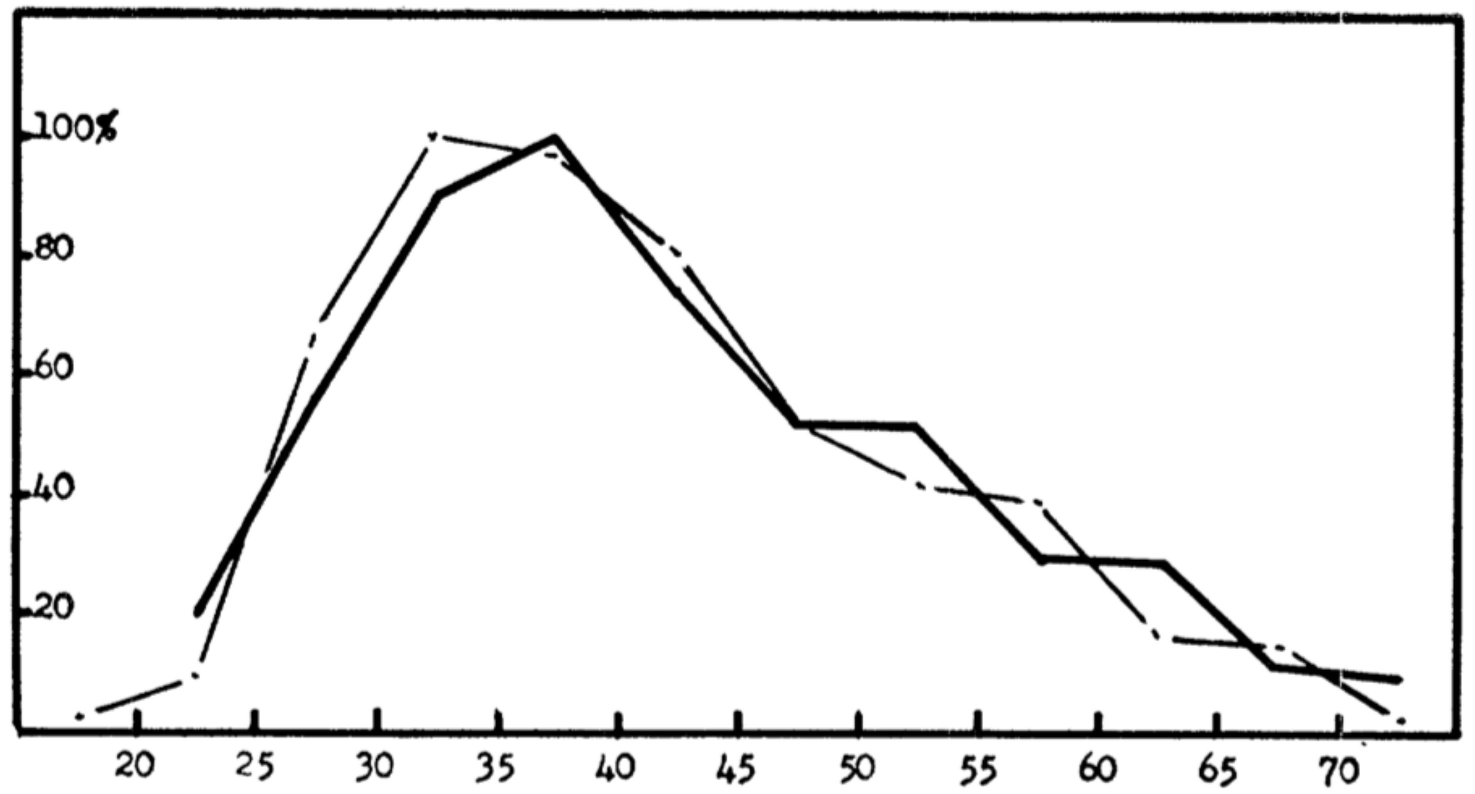

FIG. 7. Solid line: age versus creative production rate in science and mathematics for the nationals of 14 different countries other than Russia, England, France, Italy, Germany, and the U.S.A. Broken line, same as Fig. 1.

Lehman, The Scientific Monthly 78, 321-326 (1954)

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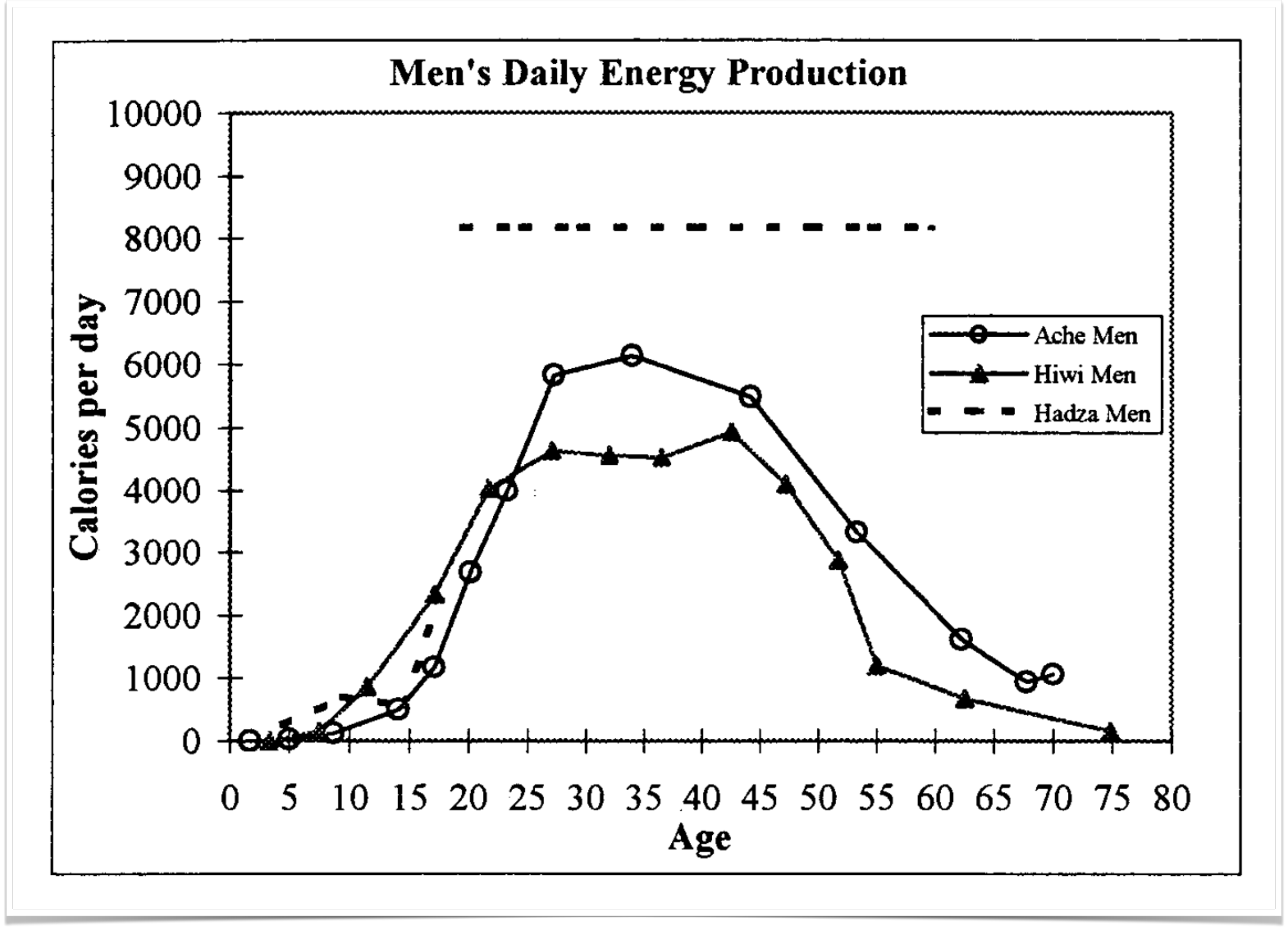
publication rates in psychology, 1986 ✓
. . . in ~~Russian~~ science & math, 1954 ✓
. . . hunter-gather groups ✓
. . . French & Philly criminals, 1835 ✓
. . . French artists, 1835 ✓
. . . many others, 1950s - present ✓



Kaplan et al., Evol. Anth.: Issues, News, and Rev., 9, 156-185 (2000)
Quetelet, 1835

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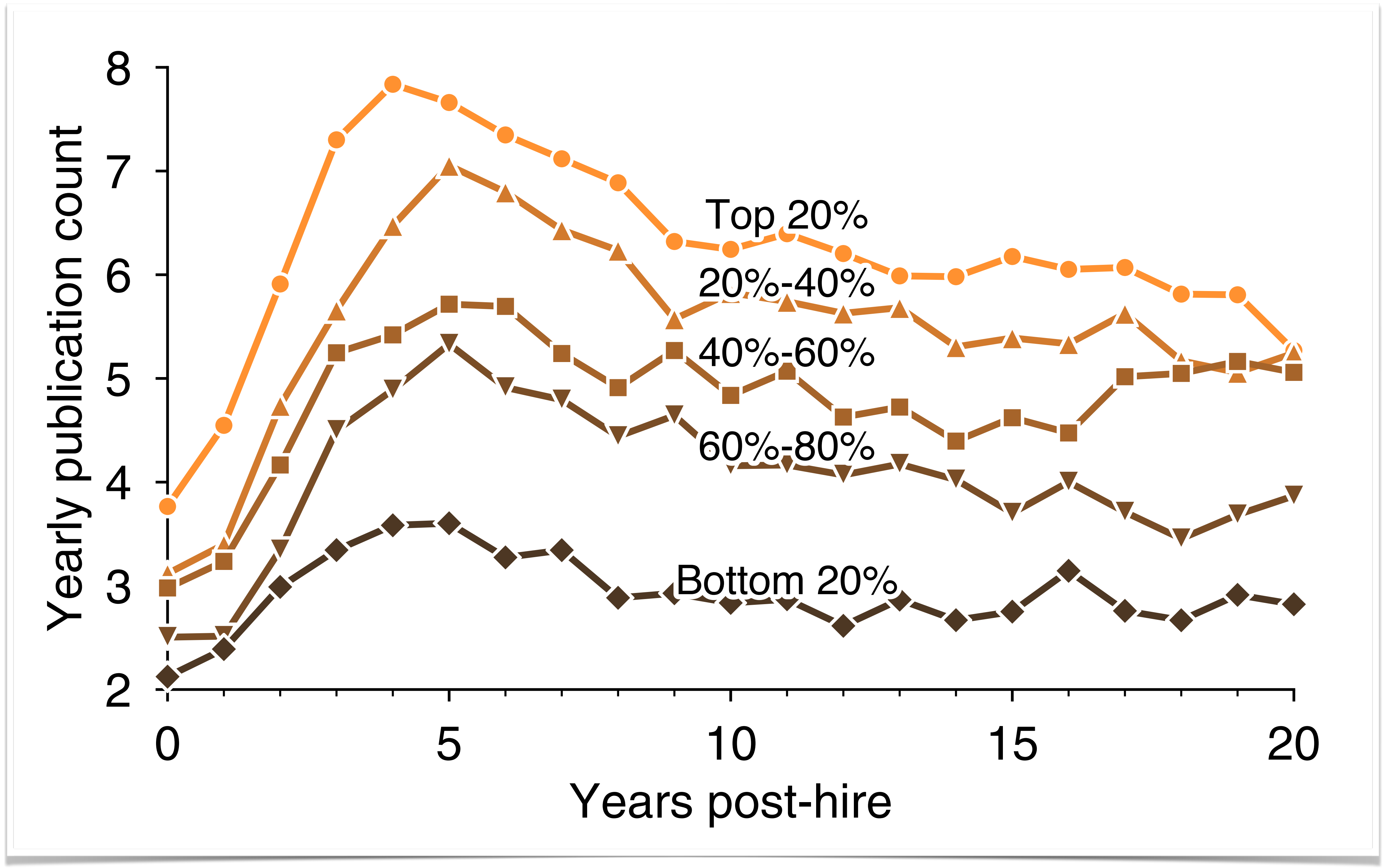
. . . **computer scientists** 👩‍💻 👨‍💻 ✓

University of Colorado Boulder
faculty hiring project

dblp
computer science bibliography



$n = 2453$ early career computer science faculty

Way, Morgan, Clauset, & Larremore, PNAS 114 (44) E9216 (2017)

productivity over a career

average productivity appears to be predictable 🔮

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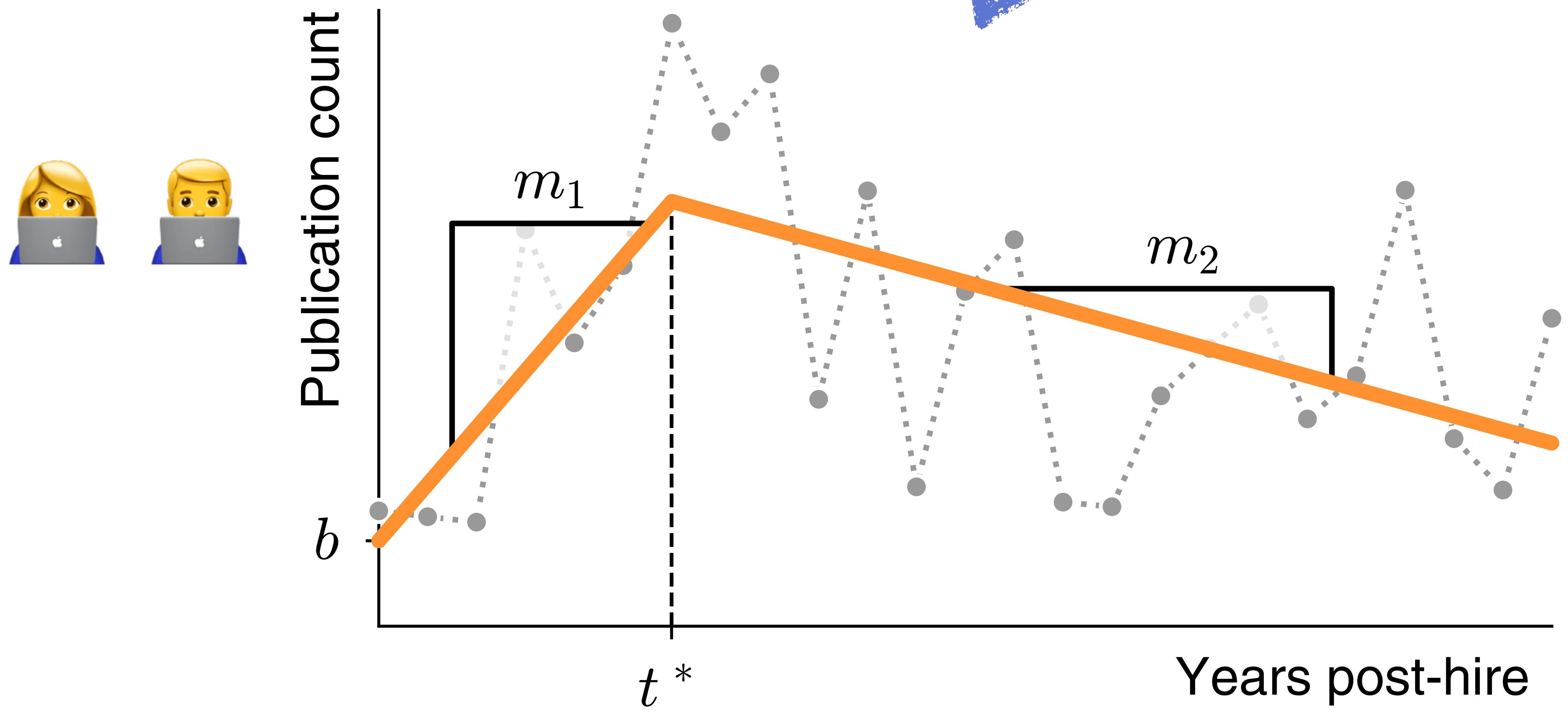

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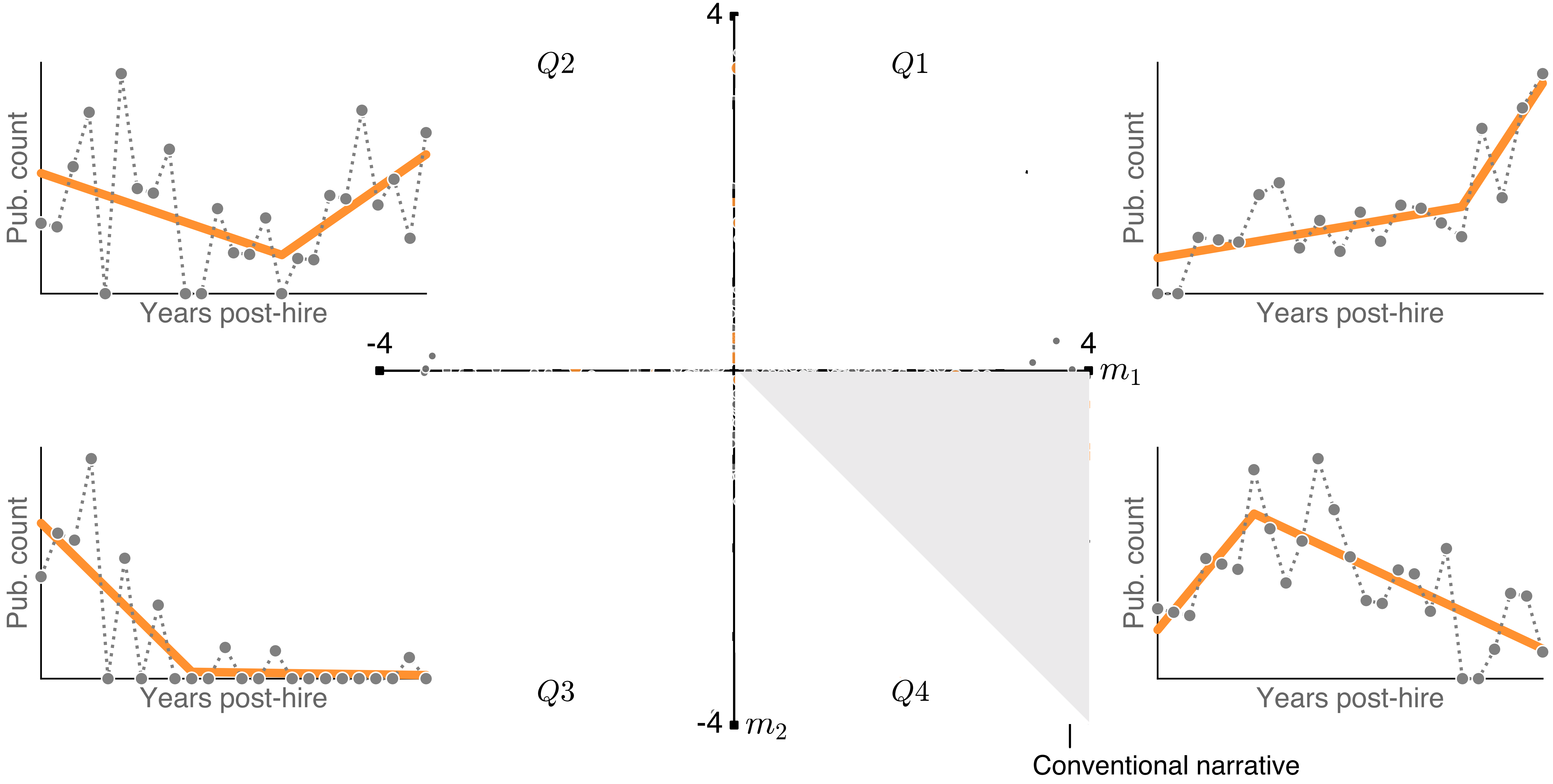

$n = 2453$ early career computer science faculty

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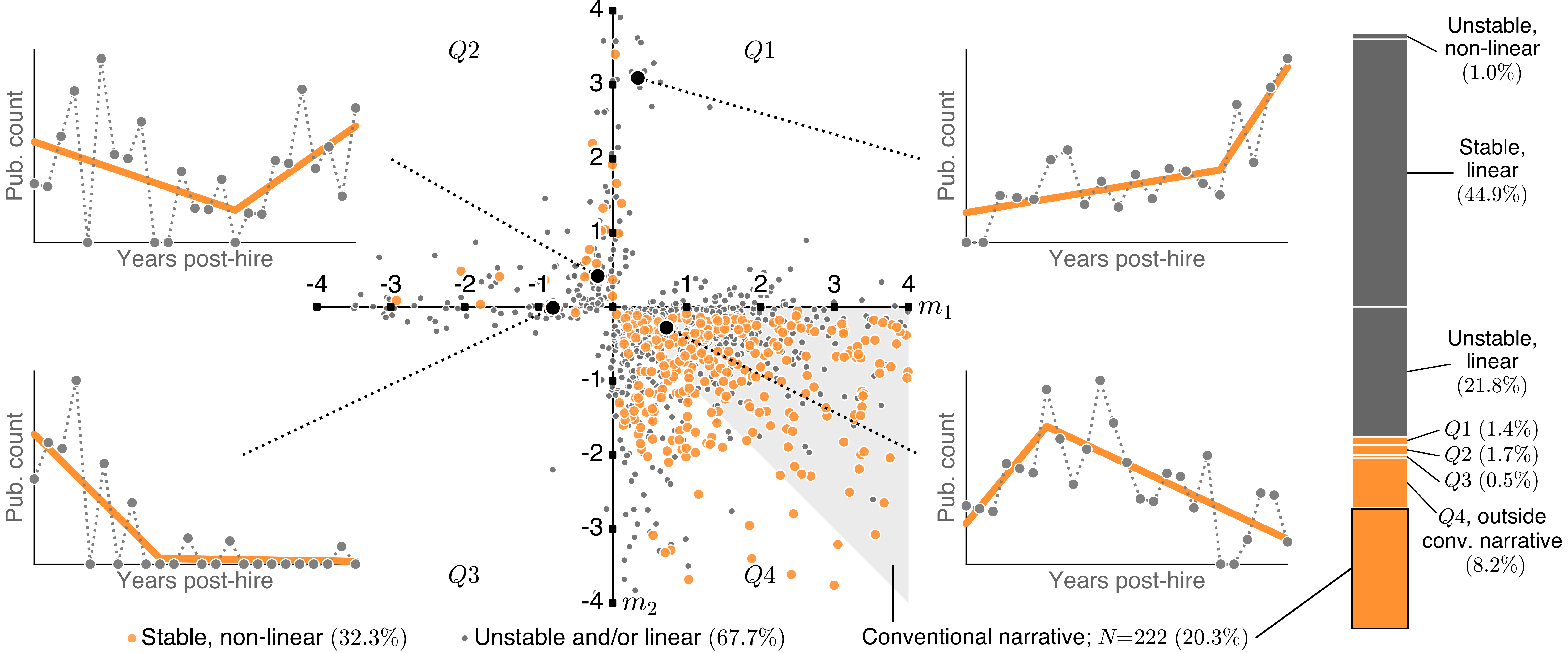
productivity over a career

average productivity appears to be predictable — **except it's not** 

- the conventional narrative only holds for 20.3% of faculty



Way, Morgan, Clauset, & Larremore, PNAS 114 (44) E9216 (2017)

timing of big discoveries

conventional narrative: *scientific creativity peaks early*

timing of big discoveries

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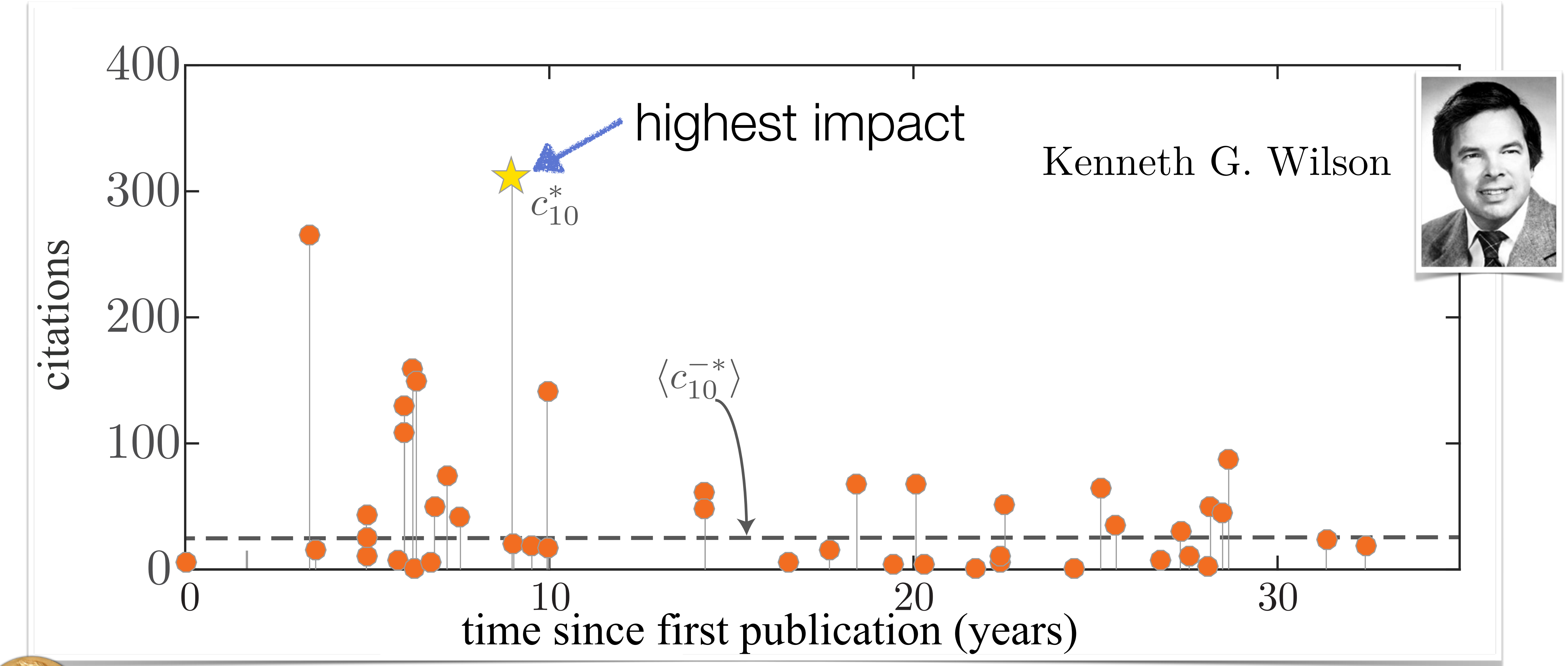
APS Data Sets for Research



Nobel in Physics (1982): phase transitions and renormalization group

450,000 articles from Physical Review, 1893-2016

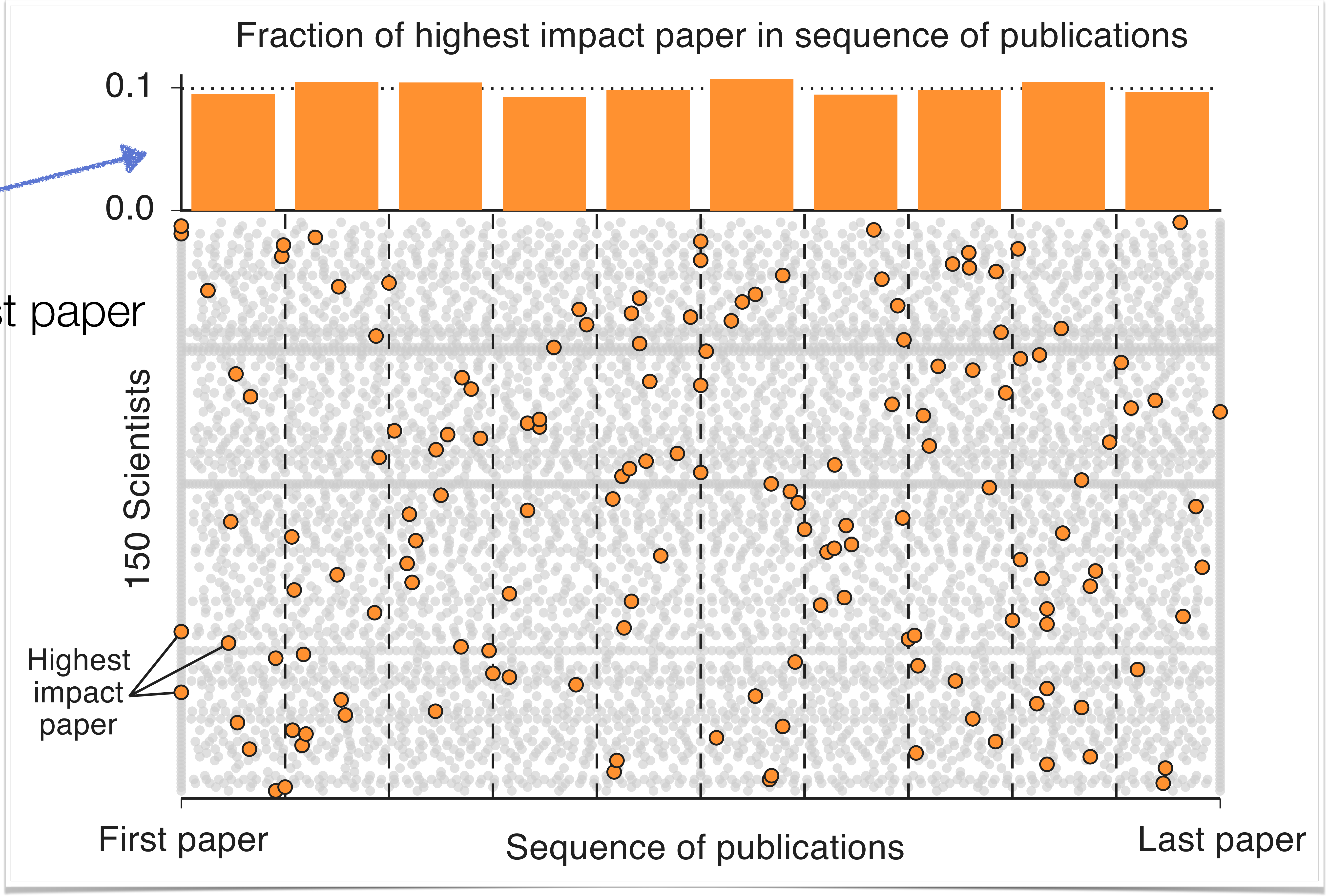
Sinatra et al., Science 354, 596 (2016)

timing of big discoveries

conventional narrative: ~~*scientific creativity peaks early*~~ — **except it doesn't** 

▶ all publications, ordered first to last

highest impact:
equally likely to be first or last paper



450,000 articles from Physical Review, 1893-2016
Sinatra et al., Science 354, 596 (2016)

predicting discoveries

some aspects of science are ***highly predictable***

- most citation counts, institution of origin, maximum impact, etc.
- aggregate trends like CPU speed, solar cell efficiency, battery cost, etc.
- interdisciplinary research is harder to publish & fund
- under-represented groups (women, non-whites) receive less funding, attention, etc.

predicting discoveries

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- aggregate trends like CPU speed, solar cell efficiency, battery cost, etc. 📈
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other aspects appear ***fundamentally unpredictable*** 🤷

- productivity over a career, timing of biggest discovery, etc.
- long-term impact of proposed project or manuscript
- what discoveries are not being made because of our focus on predictability?
- predicting discovery is just. plain. hard. (even for humans) 😊

predicting discoveries

some aspects of science are ***highly predictable*** 🔮

other aspects appear ***fundamentally unpredictable*** 🤷

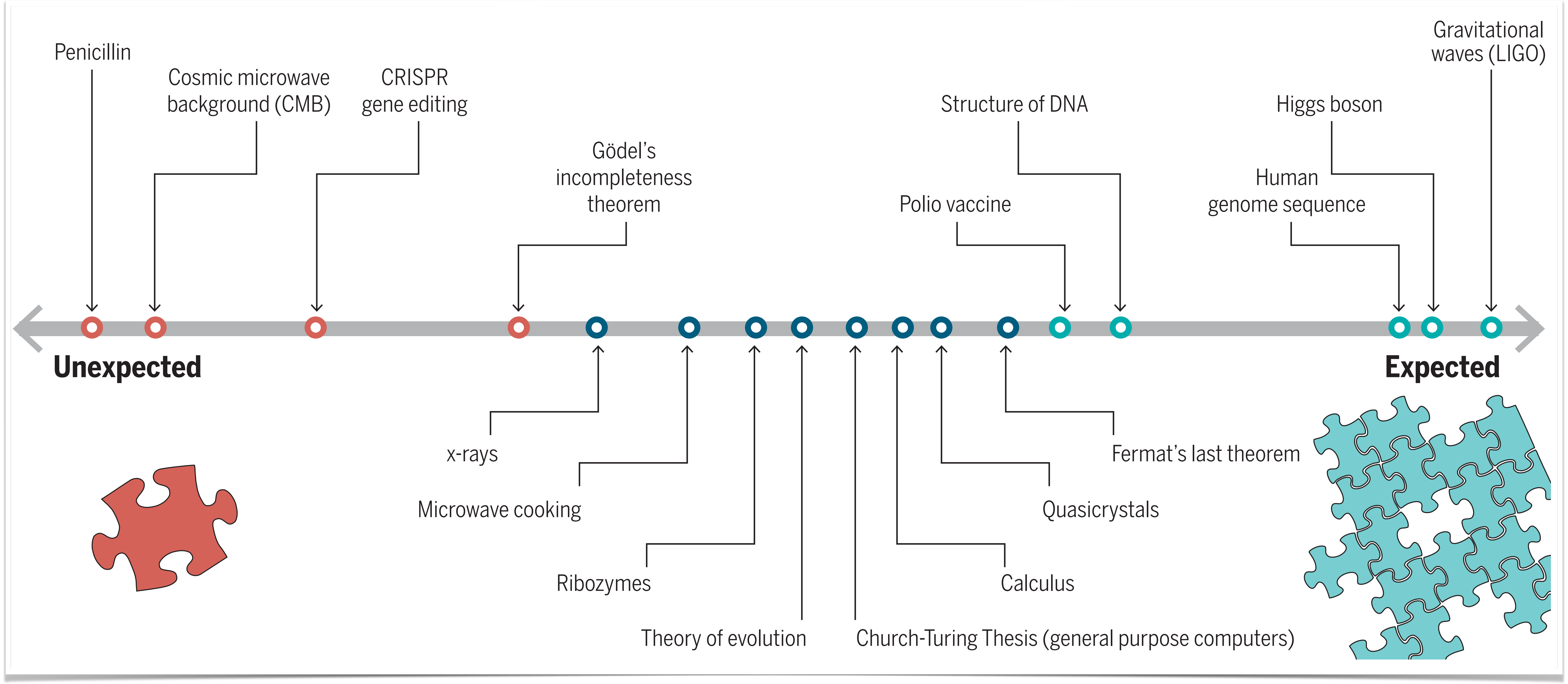
- **the data are *crude* + *biased* + *noisy* + *incomplete*** 👎
  they don't directly measure knowledge or progress
- **poor understanding of *mechanisms* that drive scientific discovery** ⚙️
  social and scientific, individual and structural
  why are some things predictable, and others not?
- **predicting *new* discoveries is a form of extrapolation = hard** 😞
  even expert humans struggle! should we expect dumb machines to do better?

looking forward

- science is a large and diverse *ecosystem*
- this diversity is a key part of its continued success
- machine learning could expand or contract it
- can we adapt diversity ideas from ecology and evolutionary theory?
  design principles of robustness, diversifying selection, stabilizing feedback, etc.
- if discovery is inherently *unpredictable*, better to cultivate a diverse scientific ecosystem than try to automate its prediction

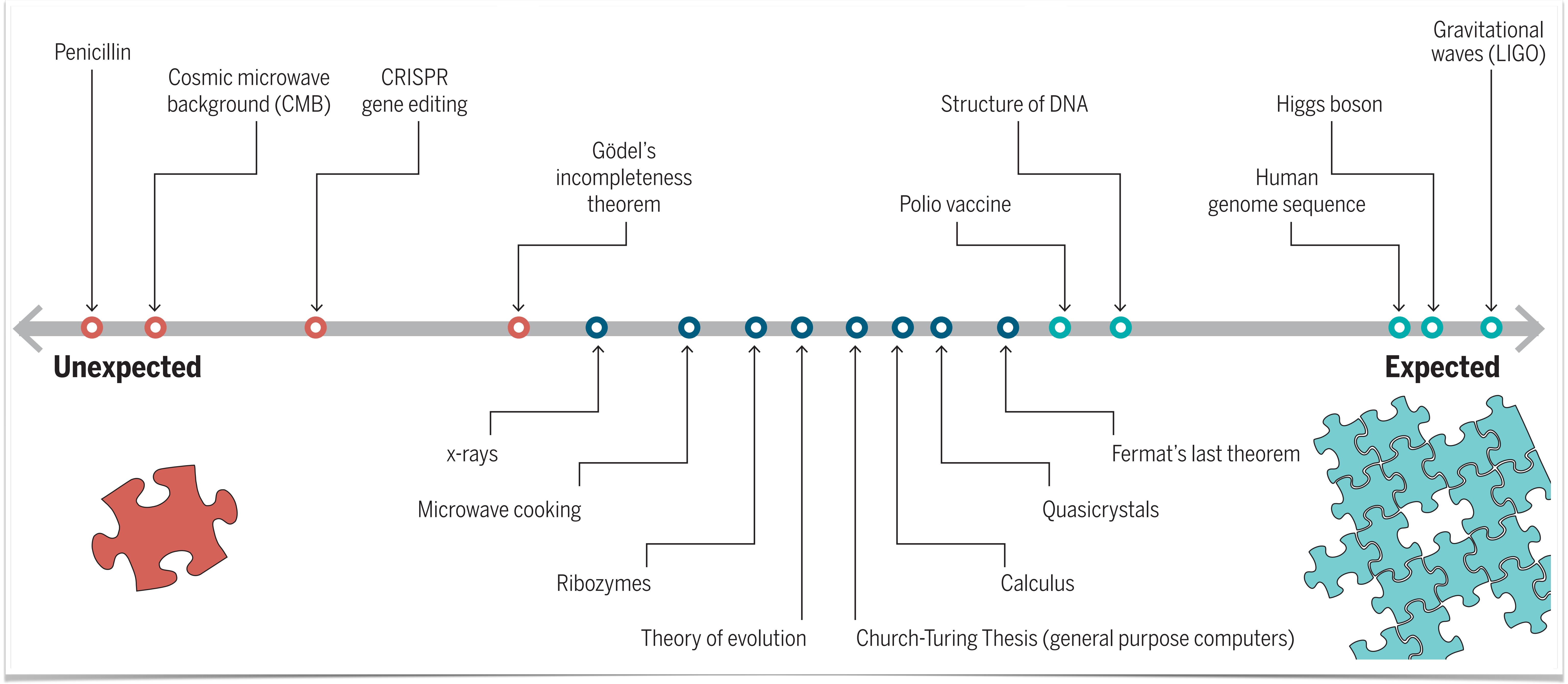
> "novel discoveries are valuable precisely because they have never been seen before, while data-driven prediction techniques can only learn about what's been done in the past"

a role for machine intelligence 🤔



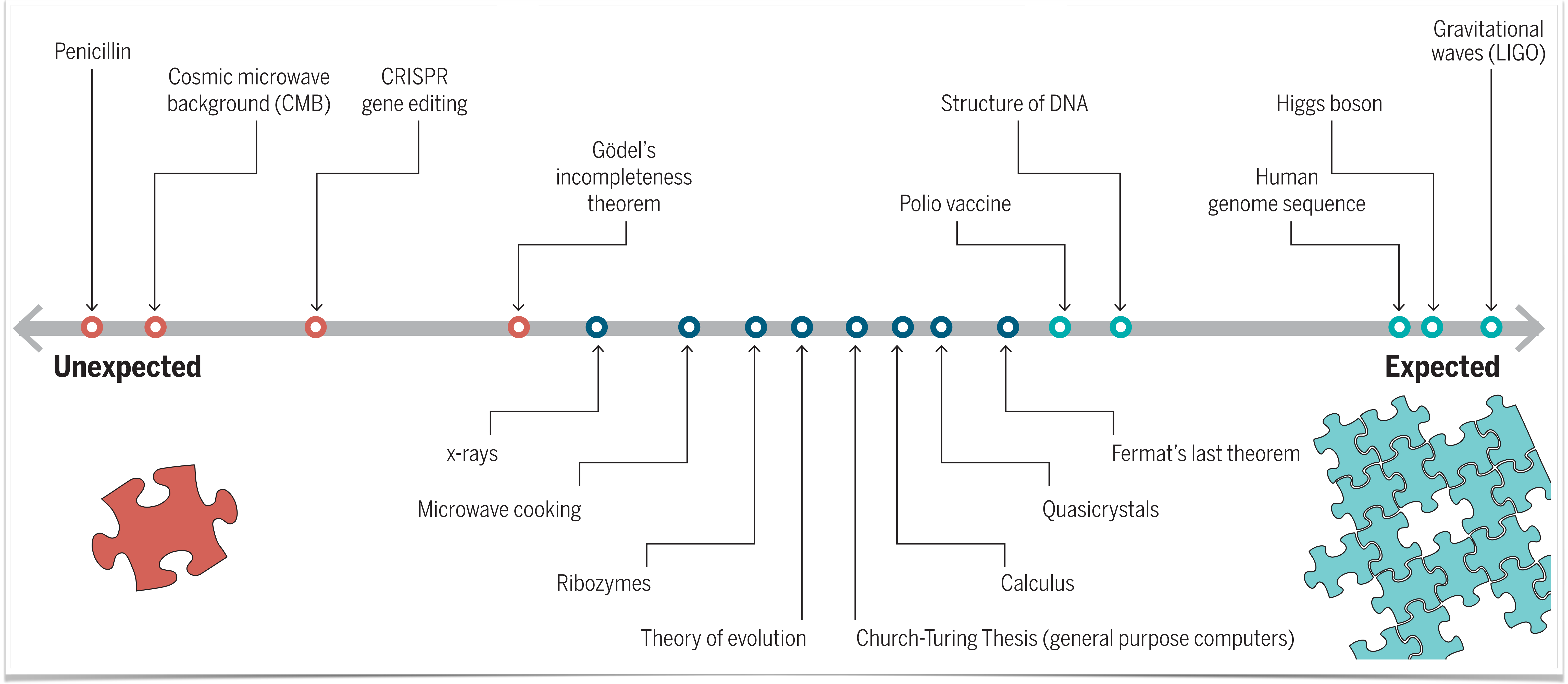
a role for machine intelligence 🤔

- knowledge production ("science") is a complex *social* system
- **probably not automatable** 🤷
  machines: *interpolation*
  science : *extrapolation*



a role for machine intelligence 🤔

- knowledge production ("science") is a complex social system
- **probably not automatable** 🤷‍♂️
  machines: *interpolation*
  science : *extrapolation*
- current AI requires huge amount of human pampering (training data, tuning, maintenance, improvement)



🤖 current AI is "dumb" = no model of mind, no physical intuition, no understanding, no *thinking*

- machines don't know *what* questions to ask = most useful for "expected" discoveries

but that's okay.

science among the machines will be a grand story of collaboration

a role for machine intelligence 🤔

- **science is probably not automatable**
  machines: *interpolation*
  science : *extrapolation*
- **solution = collaboration** 🤝
  humans : design, build, decide, interpret, extrapolate
  machines : collect, scale, calculate, estimate, interpolate
- **hybrid approaches** will extend human control of natural and artificial processes in seemingly magical ways and *it will change humans in the process* 💁 + 🤖
- **a secret**: this is history! 📜 not the future.

  every revolutionary technology has been a super power that changes humans: 🦸 🦸‍♀️

  language 💬, writing ✍️, mathematics ♾️, democracy 🏛️, science 🔬, computers 💻…

looking forward (again)

- science is a large and diverse *ecosystem*
- this diversity is a key part of its continued success
- machine learning could expand or contract it
- can we adapt diversity ideas from ecology and evolutionary theory?
  design principles of robustness, diversifying selection, stabilizing feedback, etc.
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> "novel discoveries are valuable precisely because they have never been seen before, while data-driven prediction techniques can only learn about what's been done in the past"

SPECIAL SECTION PREDICTION

ESSAY

Data-driven predictions in the science of science

Aaron Clauset,[1,2]* Daniel B. Larremore,[2] Roberta Sinatra[3,4]

Science 355, 477-480 (2017)

Prof. Aaron Clauset (Colorado)

Prof. Daniel B. Larremore (Colorado)

Prof. Roberta Sinatra (ITU Copenhagen)

PNAS

The misleading narrative of the canonical faculty productivity trajectory

Samuel F. Way[a,1], Allison C. Morgan[a], Aaron Clauset[a,b,c,2], and Daniel B. Larremore[a,b,c,1,2]

[a]Department of Computer Science, University of Colorado, Boulder, CO 80309; [b]BioFrontiers Institute, University of Colorado, Boulder, CO 80303; and [c]Santa Fe Institute, Santa Fe, NM 87501

PNAS 114 (44) E9216 (2017)

Dr. Samuel F. Way (Colorado)

Dr. Allison C. Morgan (Colorado)

see also:

Morgan et al. "The unequal impact of parenthood in academia." *Science Advances* 7 (2021)

Way et al., "Productivity, prominence, and the effects of academic environment." *PNAS* 116 (2019)

Morgan et al., "Prestige drives epistemic inequality in the diffusion of scientific ideas." *EPJ Data Science* 7 (2018)

Way et al., "Gender, productivity, and prestige in computer science faculty hiring networks." *Proc. WWW* (2016)

Clauset et al., "Systematic inequality and hierarchy in faculty hiring networks." *Science Advances* 1 (2015)

NSF

🤔 Questions?