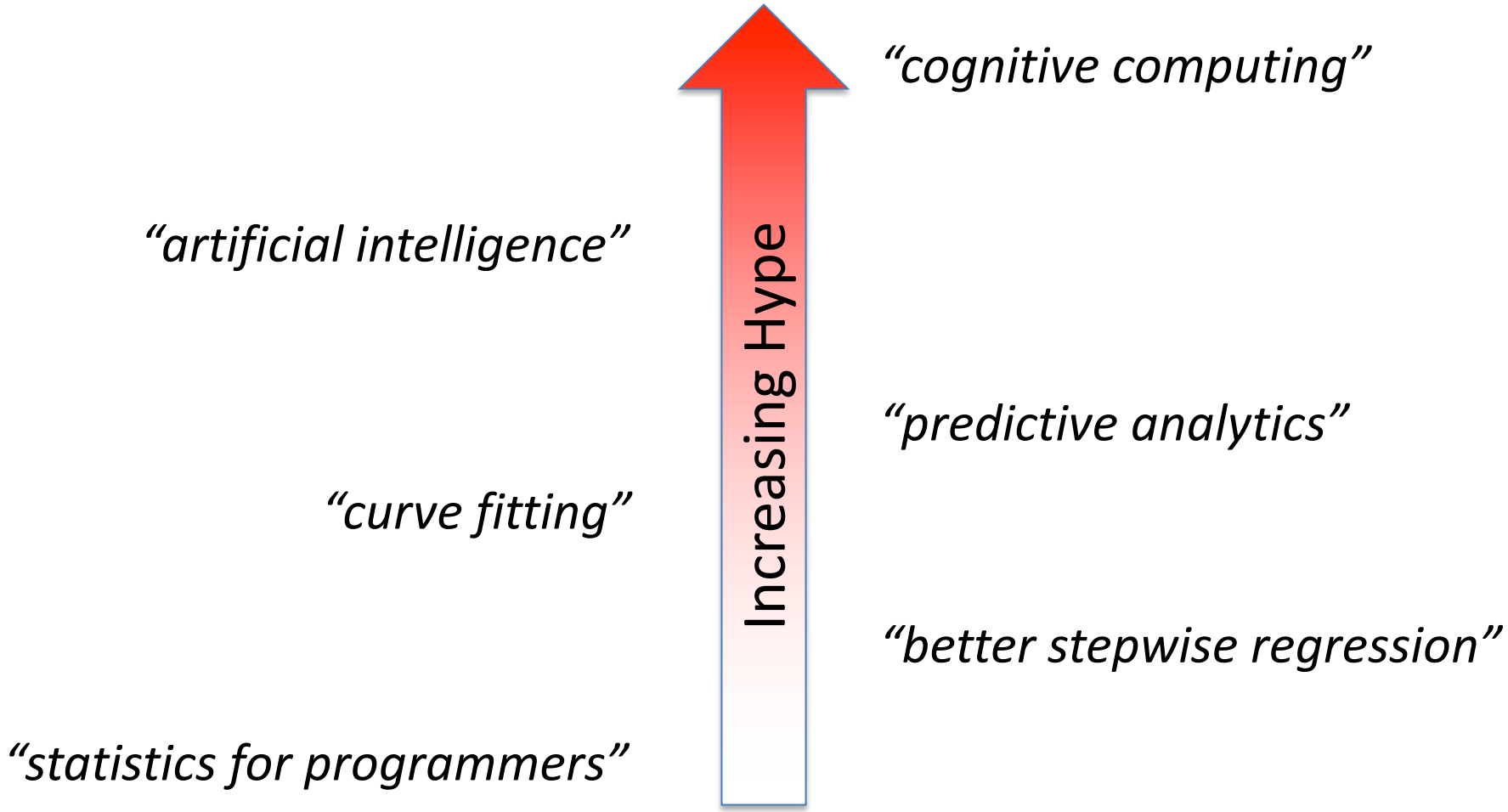
Principles and Culture of Data Science

May 30, 2020

Lecture 2, Applied Data Science
MMCi Term 4, 2020

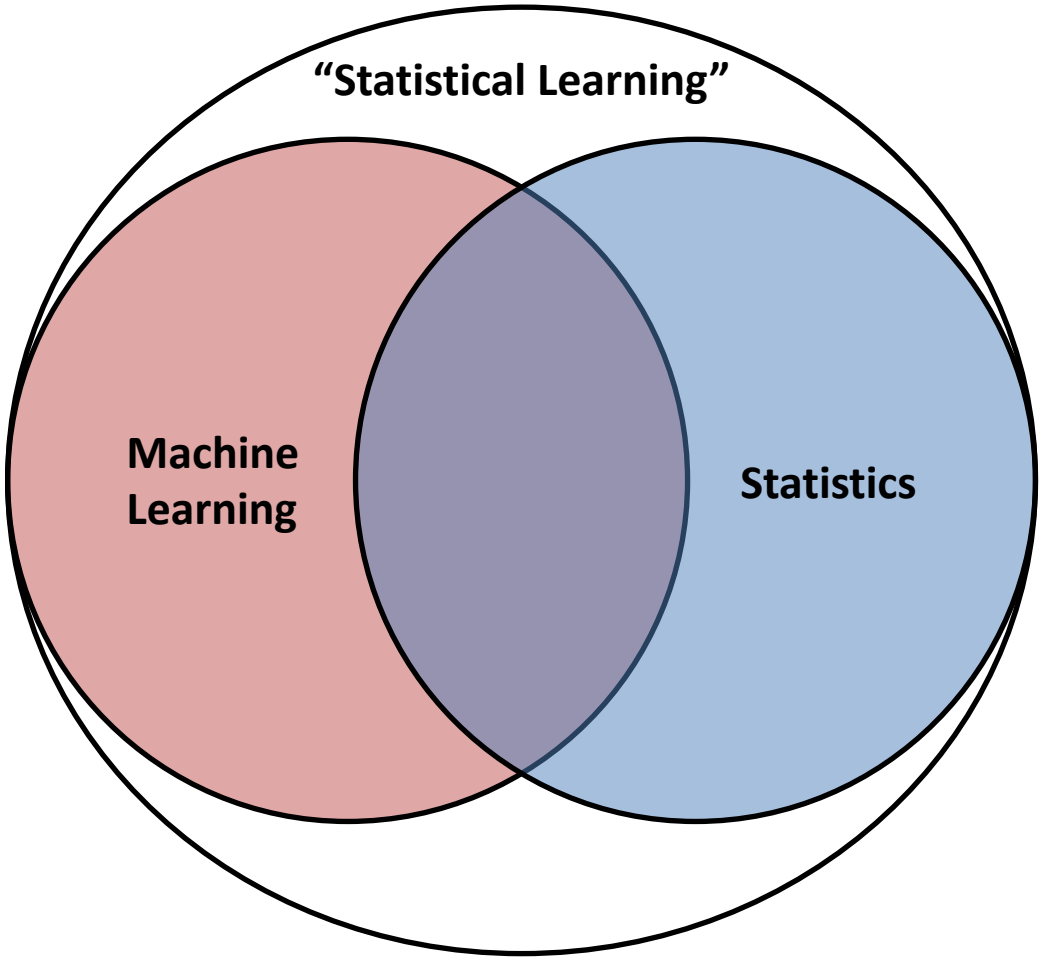
Matthew Engelhard

What are Machine Learning and Data Science?



Q: What is Machine Learning?

"ML is an algorithmic field that blends ideas from statistics, computer science and many other disciplines to design algorithms that process data, make predictions and help make decisions" – M. I. Jordan



- Can’t squeeze information that doesn’t exist out of a dataset
- So, scientific and clinical judgement remain critical to success

“BIG DATA”: DISTINCTION OR MEME?


4 September 2008 | www.nature.com/nature | £10
THE INTERNATIONAL WEEKLY JOURNAL OF SCIENCE
nature
THE BITER BIT
Viral infections for viruses
TROPICAL CYCLONES
The strong get stronger
BLACK HOLE PHYSICS
A new window on the Galactic Centre
BIG DATA

Epic

Big Data

Long Data

- Large *N*
- A clinical study with 50k participants
- A speech database with 10M short recordings

Wide Data

- Large *M*
- A mHealth study with 6 months of wearables data in 20 participants
- 10 minutes of raw fMRI data in 8 participants

“Big Data”: Distinction or Meme?

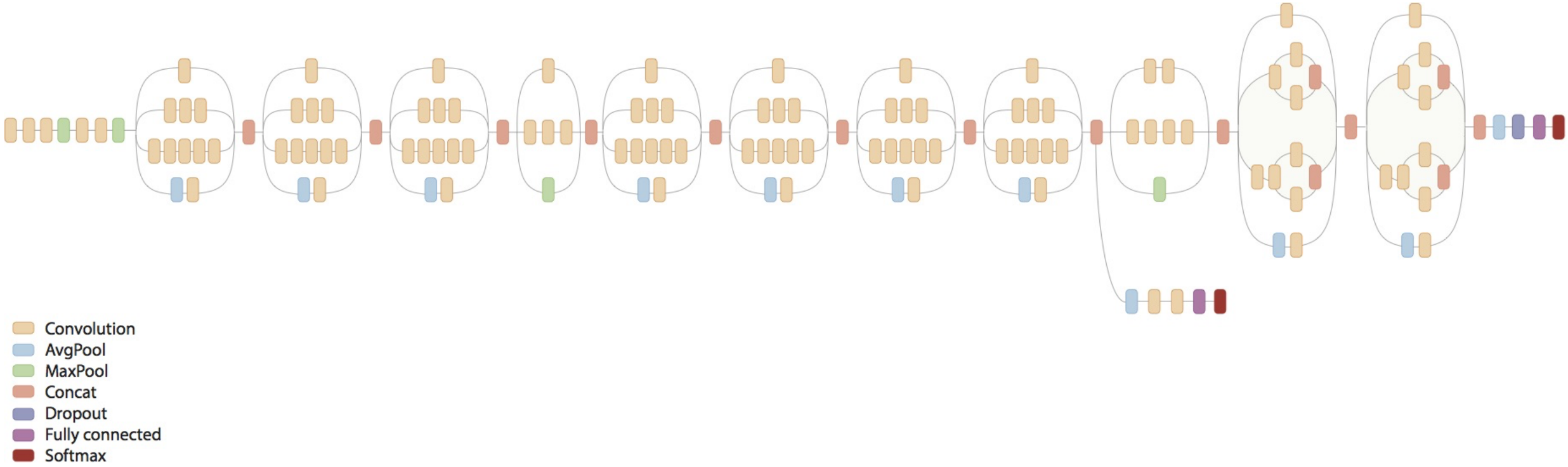
“We can immediately reject ‘big data’ as a criterion for meaningful distinction between statistics and data science”

-- David Donoho, *50 years of Data Science*

His points:

- Statisticians have been looking at big data, e.g. census data, for >200 years.
- Statisticians have long studied sampling and sufficient statistics, which allow them to work with big datasets

Neural networks thrive on big data



Inception v3 Convolutional Neural Network

Hardware and computational platforms for big data and deep learning

Edward

TensorFlow

Keras

PREDICTIVE MODELING CULTURE

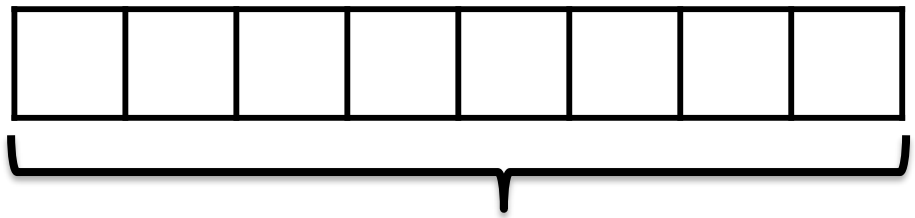
Previous Example: ICU Mortality Prediction

- Outcome:

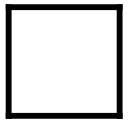
$$y_i = \begin{cases} 1, \text{patient } i \text{ dies} \\ 0, \text{patient } i \text{ lives} \end{cases}$$

- Features: On admission, what is patient i's

$$\{\text{age, sex, temperature, blood pressure, ...}\}$$



x_i, features for patient i



y_i, did patient i die

Previous Example: ICU Mortality Prediction

- Outcome: $$y_i = \begin{cases} 1, \text{patient } i \text{ dies} \\ 0, \text{patient } i \text{ lives} \end{cases}$$
- Features: On day i what is the
  $\{1: \text{age}, 2: \text{sex}, 3: \text{ temperature}, 4: \text{blood pressure} \ldots\}$

$$z_i = b_1 x_{i1} + b_2 x_{i2} + \cdots + b_M x_{iM} + b_0$$

Age

Blood Pressure

- If increased age increases odds of mortality, b_1 should be positive

What's our goal?

- **Answer 1: Determine who's at highest risk of death so we can plan or manage resources accordingly**

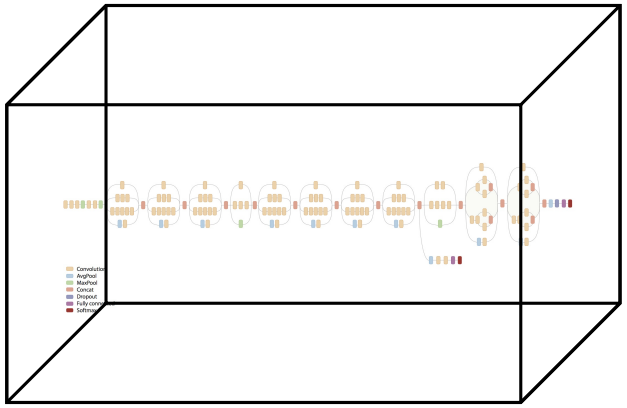
- **Answer 2: Identify predictors of mortality to further scientific understanding and design interventions**

Machine Learning: A Black Box?

What's our goal?

- **Answer 1: Determine who's at highest risk of death so we can plan or manage resources accordingly**

- **Answer 2: Identify predictors of mortality to further scientific understanding and design interventions**

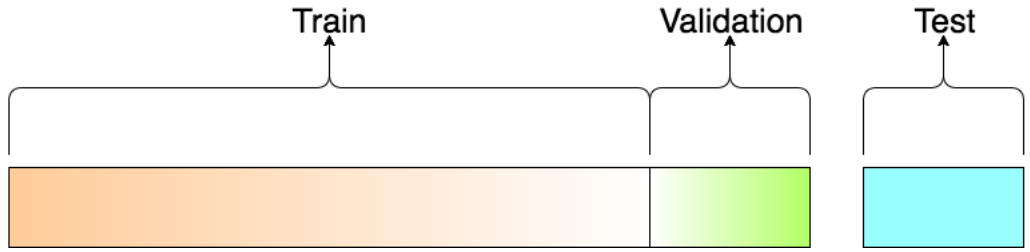


What's our goal?

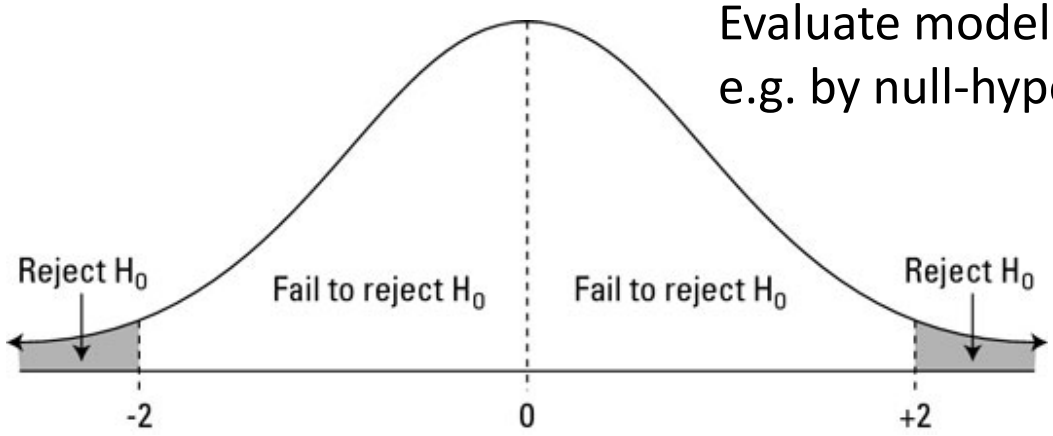
- **Answer 1: Determine who's at highest risk of death so we can plan or manage resources accordingly**

- **Answer 2: Identify predictors of mortality to further scientific understanding and design interventions**

DS evaluation:
Determine whether the model performs well on new data



Explanatory Approach:
Evaluate model parameters, e.g. by null-hypothesis testing



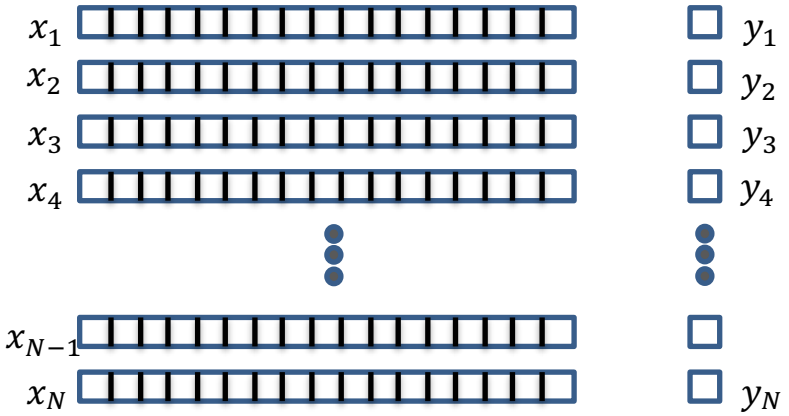
The Secret Sauce of Predictive Modeling?

THE COMMON TASK FRAMEWORK

- Ingredient 1: Standardized evaluation of model performance

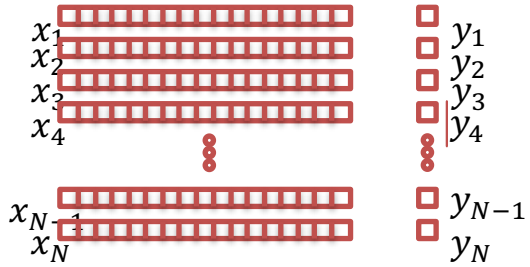
Standardized Evaluation Strategy

- We want to know how the network will perform *in the real world*
- So, we try it with new data
- This is costly; instead, can we use existing data to estimate performance?



Training Set

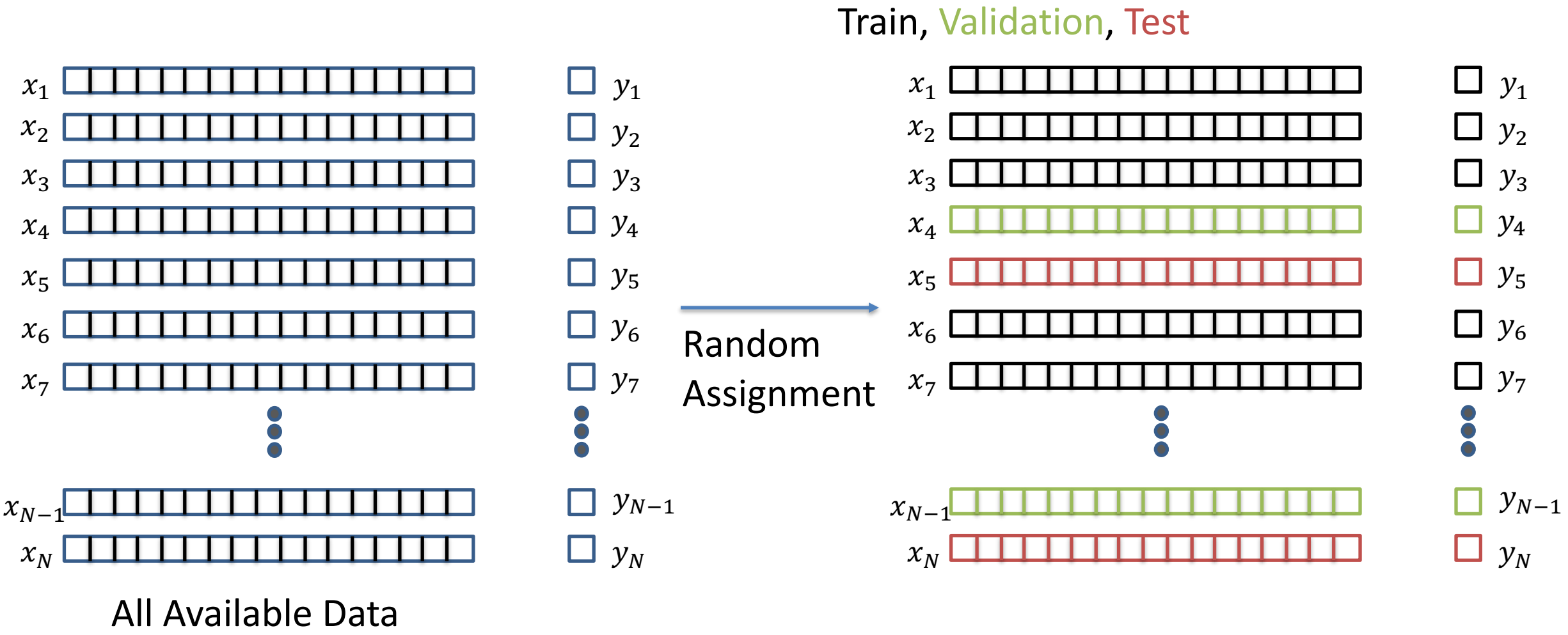
$(b_0, b_1, \ldots b_M)$



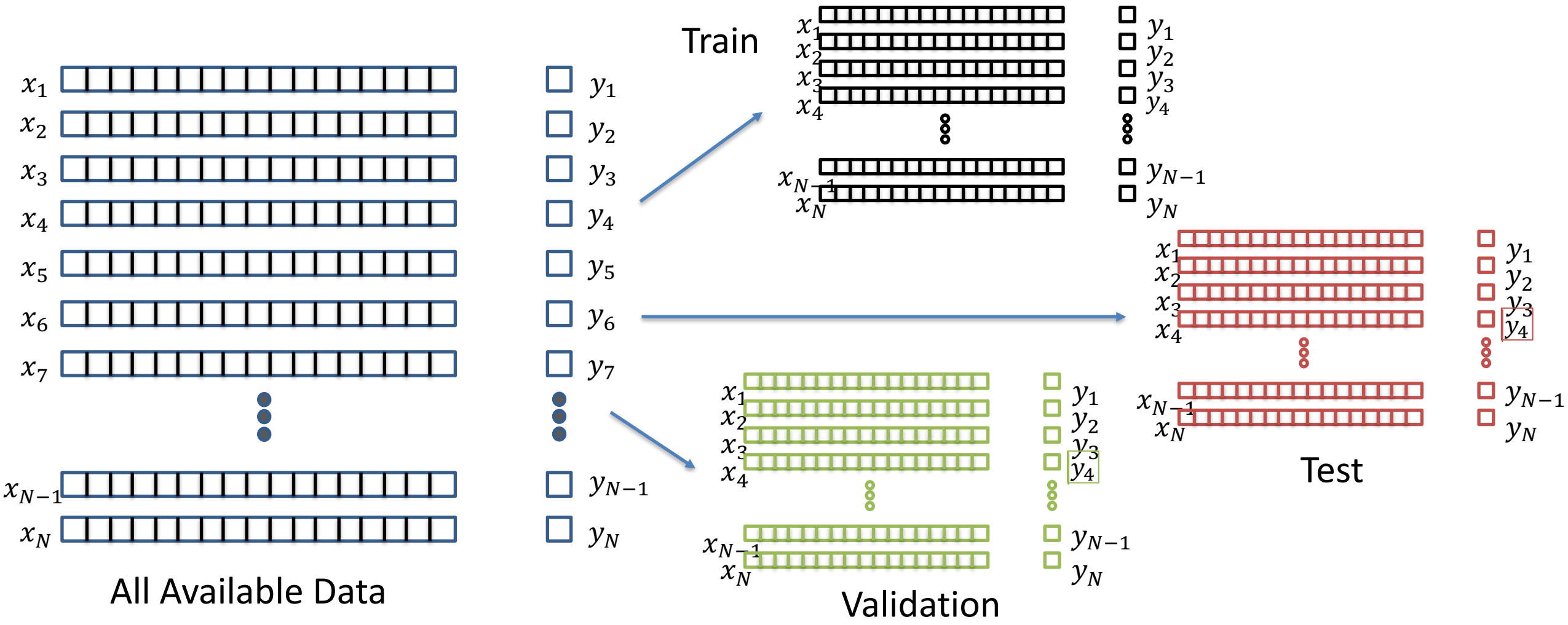
"New" Real-World Data

Estimate Real-World Performance

Split Data into Separate Groups



Split Data into Separate Groups

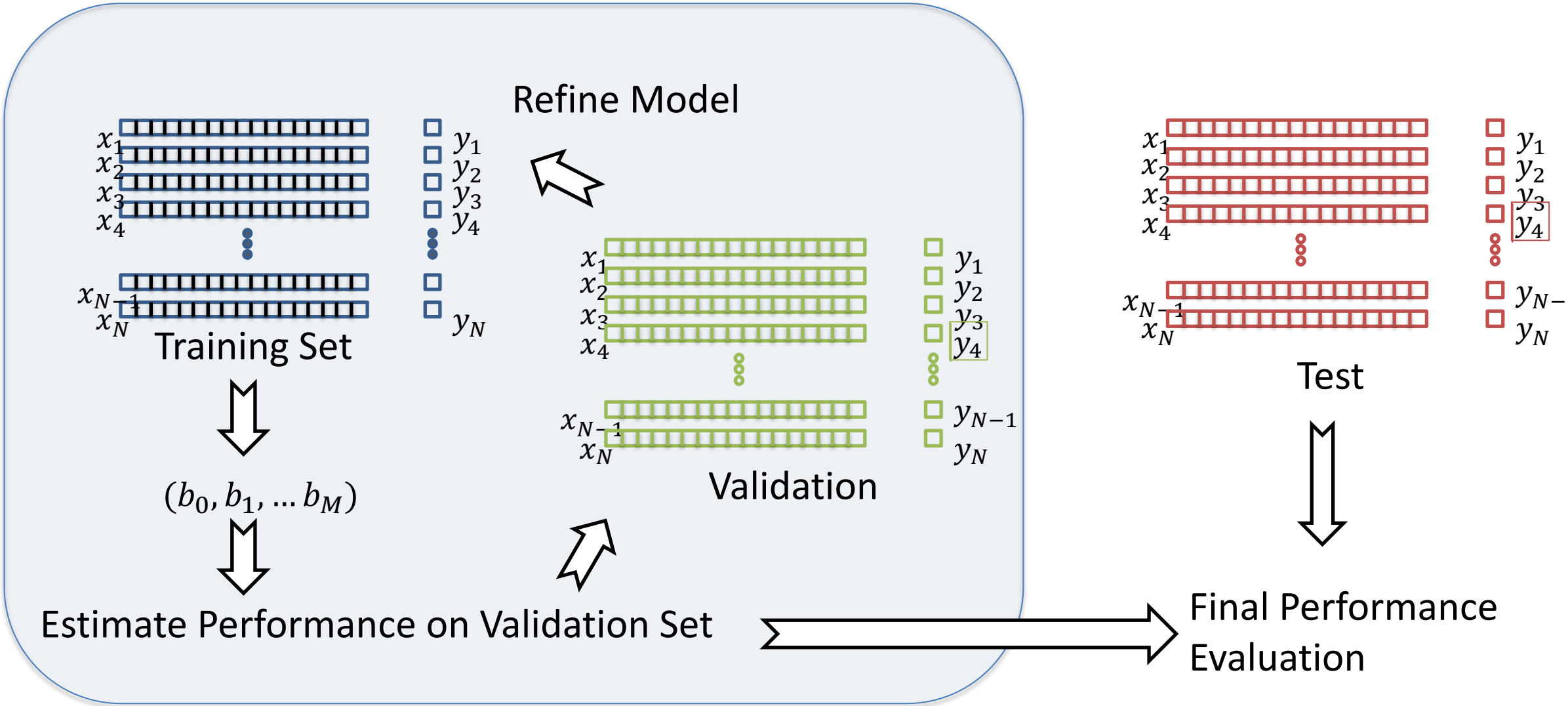


Test set

- This should be set aside prior to any analysis, and **will not be used to learn or fit any parameters**
- After learning the model, we evaluate its performance on the test set
  - This data was not included in the training/fitting, so it is analogous to running a new synthetic experiment
- Ideally, the test set will be used *once*.
  - Reusing the test set leads to bias; performance estimates will be optimistic
- So, how do we compare different models?

Validation (or *Tuning*) Set

- Want to be able to compare which approach is best
  - Problematic if we only want to use a test set once
  - Can create a second held-out dataset
- The validation data is not used for learning parameters, but can be used repeatedly to estimate performance of a model
- We can pick the model with the best performance on the validation set, and run a final evaluation on the test data


Refine Model
x_1 x_2 x_3 x_4 x_{N-1} x_N
y_1 y_2 y_3 y_4 y_N
Training Set
$(b_0, b_1, \ldots b_M)$
x_1 x_2 x_3 x_4 x_{N-1} x_N
y_1 y_2 y_3 y_4 y_{N-1} y_N
Validation
Estimate Performance on Validation Set
x_1 x_2 x_3 x_4 x_{N-1} x_N
y_1 y_2 y_3 y_4 y_{N-1} y_N
Test
Final Performance Evaluation

Pitfalls: Training, Validation, and Test

This can be more nuanced than it might seem,
and is a common source of methodological errors!

- Pitfall 1: Multiple data points from the same individual or source
- Pitfall 2: Utilizing data from the test or validation set prior to "modeling"
  - feature selection using the whole dataset
  - other information "leaks"
- Pitfall 3: Systematic differences between test, validation, and training sets

Pitfalls: Training, Validation, and Test

This can be more nuanced than it might seem,
and is a common source of methodological errors!

- PITFALL 0: Repeatedly evaluating on the test set!

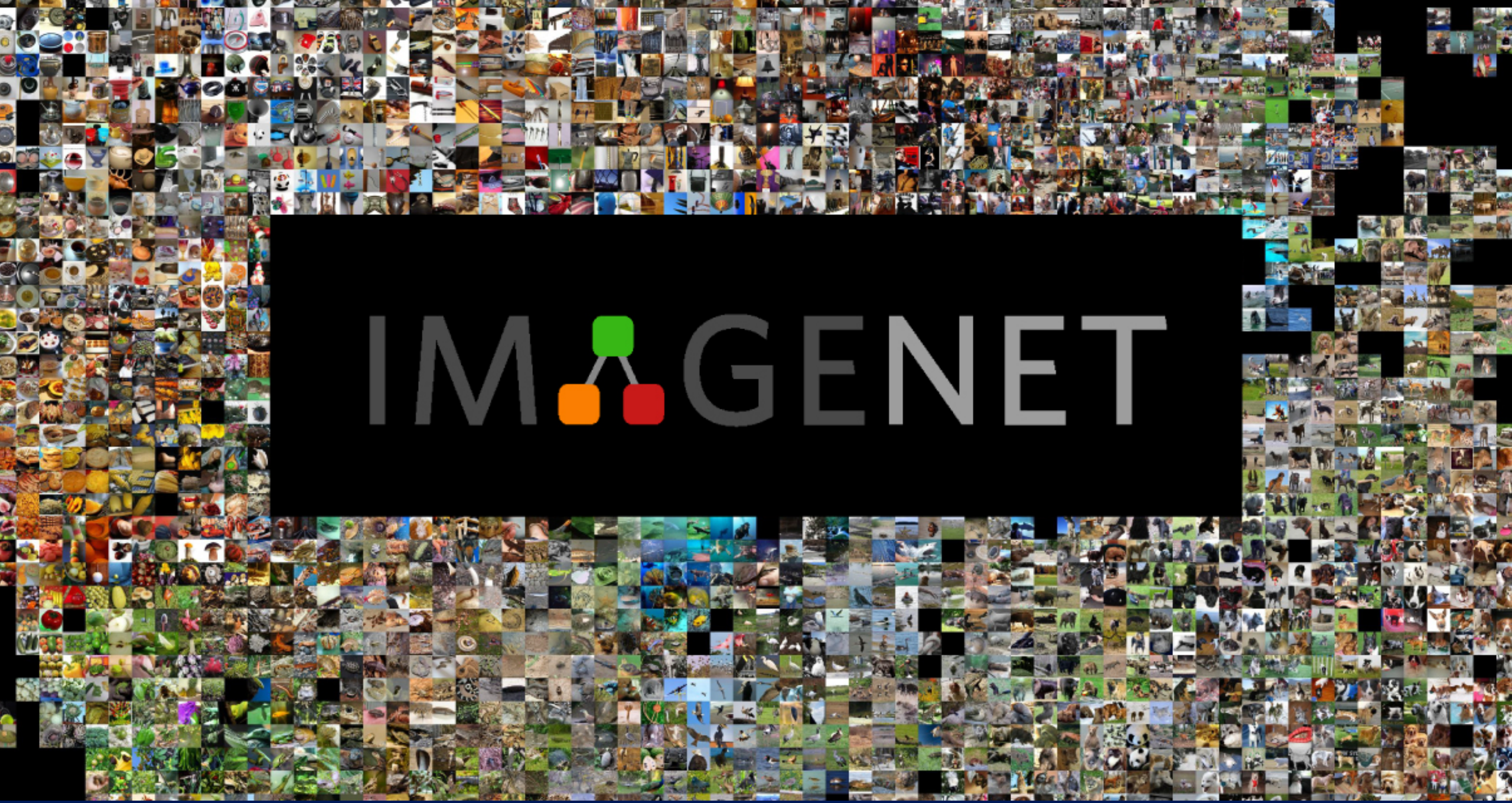
- Pitfall 1: Multiple data points from the same individual or source

- Pitfall 2: Utilizing data from the test or validation set prior to "modeling"
  - feature selection using the whole dataset
  - other information "leaks"

- Pitfall 3: Systematic differences between test, validation, and training sets

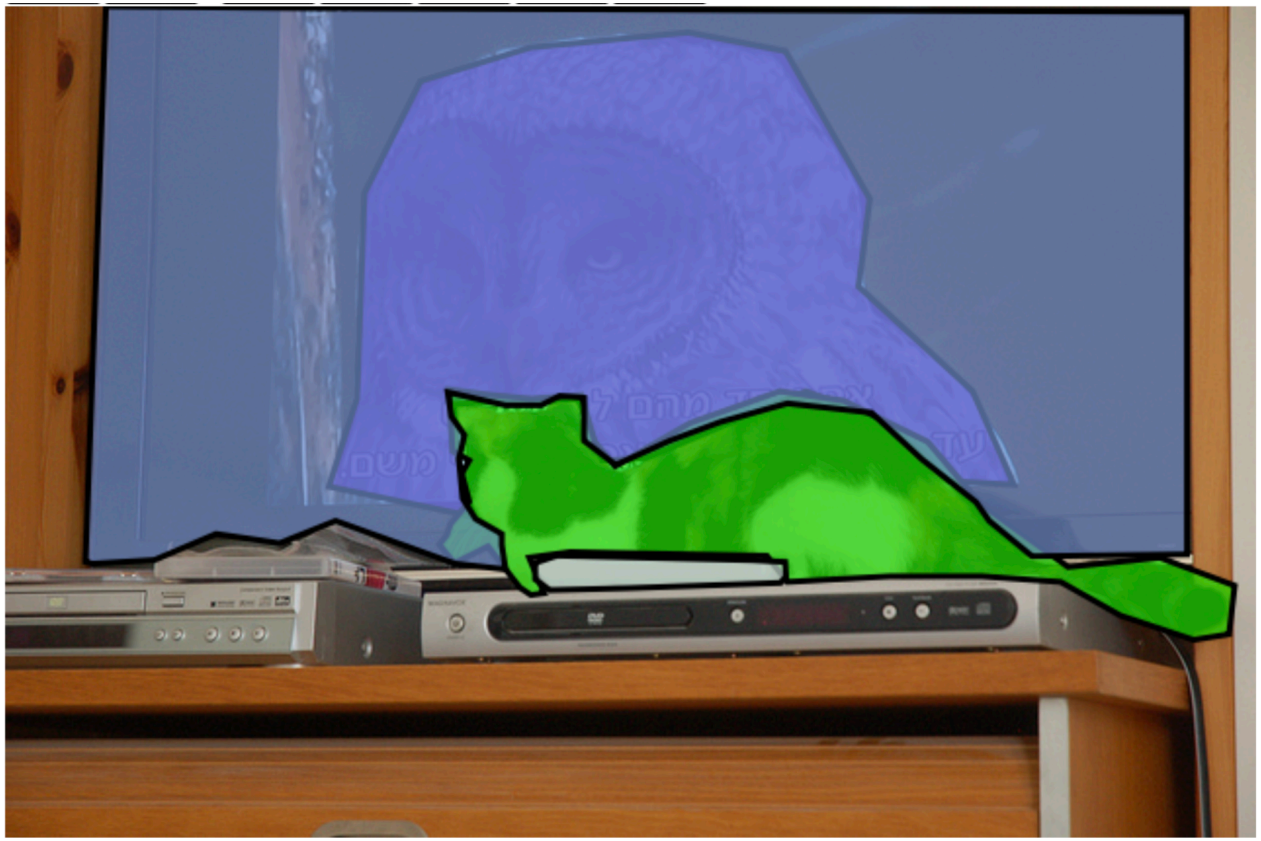
- Ingredient 1: Standardized evaluation of model performance

- Ingredient 2: Publicly-available training datasets


IMAGENET

COCO

Common Objects in Context



Stanford Question Answering Dataset (SQuAD 2.0)

Microorganisms or toxins that successfully enter an organism encounter the cells and mechanisms of the innate immune system. The innate response is usually triggered when microbes are identified by pattern recognition receptors, which recognize components that are conserved among broad groups of microorganisms, or when damaged, injured or stressed cells send out alarm signals, many of which (but not all) are recognized by the same receptors as those that recognize pathogens. Innate immune defenses are non-specific, meaning these systems respond to pathogens in a generic way. This system does not confer long-lasting immunity against a pathogen. The innate immune system is the dominant system of host defense in most organisms.

What part of the innate immune system identifies microbes and triggers immune response?
Ground Truth Answers: pattern recognition receptors | receptors | cells
Prediction: pattern recognition receptors

For most organisms, what is the dominant system of defense?
Ground Truth Answers: innate immune system | innate immune system | The innate immune
Prediction: The innate immune system

Pattern recognition receptors recognize components present in broad groups of what?
Ground Truth Answers:
microorganisms | microorganisms | microorganisms
Prediction: microorganisms

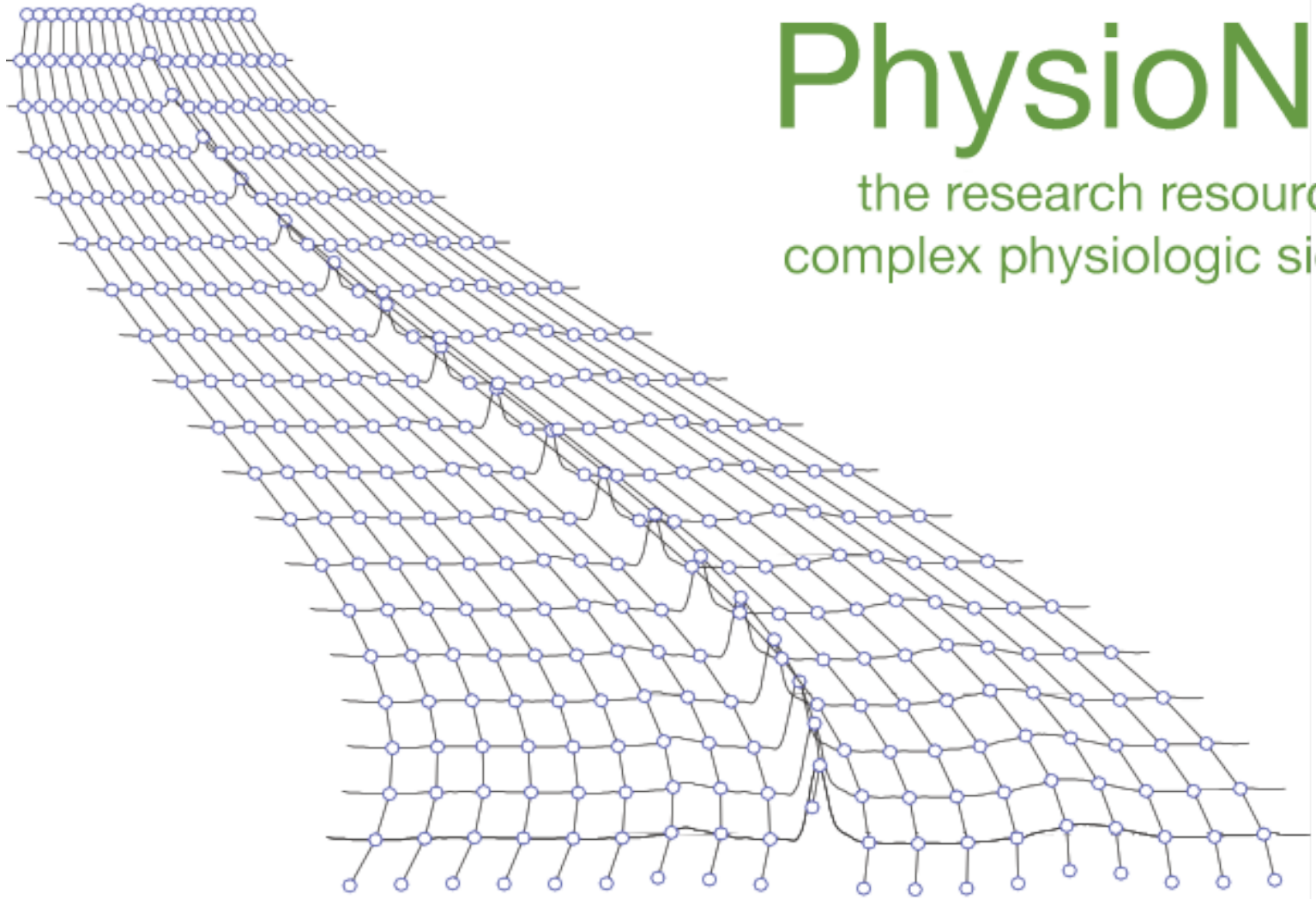
The innate immune system responds in a generic way, meaning it is what?
Ground Truth Answers: non-specific | non-specific | non-specific
Prediction: non-specific

Amazon Reviews Dataset


```
{"reviewerID": "A2SUAM1J3GNN3B",
 "asin": "0000013714",
 "reviewerName": "J. McDonald",
 "helpful": [2, 3],
 "reviewText":
        "I bought this for my husband who plays the
        piano. He is having a wonderful time playing these
        old hymns. The music is at times hard to read
        because we think the book was published for singing
        from more than playing from. Great purchase
        though!",
 "overall": 5.0,
 "summary": "Heavenly Highway Hymns",
 "unixReviewTime": 1252800000,
 "reviewTime": "09 13, 2009”}
```

If you use MIMIC data or code in your work, please cite the following publication:

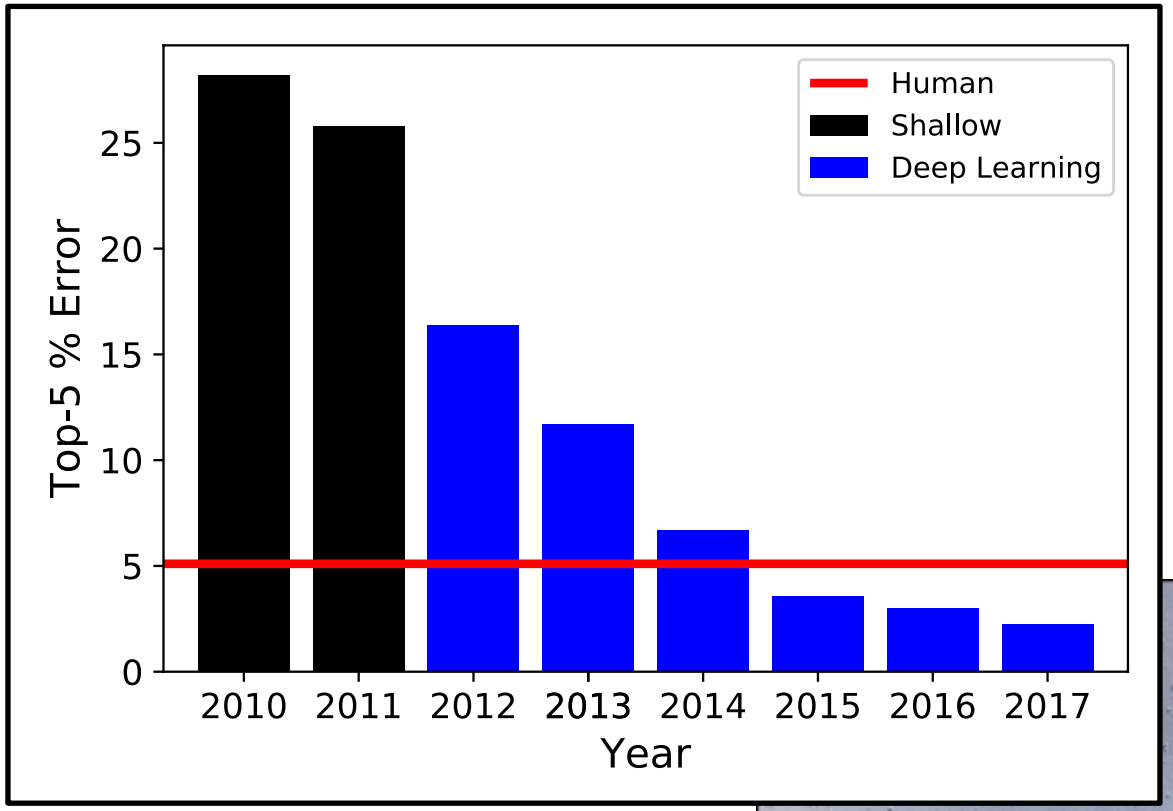
MIMIC-III, a freely accessible critical care database. Johnson AEW, Pollard TJ, Shen L, Lehman L, Feng M, Ghassemi M, Moody B, Szolovits P, Celi LA, and Mark RG. Scientific Data (2016). DOI: 10.1038/sdata.2016.35.
Available from: http://www.nature.com/articles/sdata201635



PhysioNet

the research resource for
complex physiologic signals

- Ingredient 1: Standardized evaluation of model performance
- Ingredient 2: Publicly-available training datasets
- Ingredient 3: Competition with Impartial Scoring


Human
Shallow
Deep Learning
Top-5 % Error
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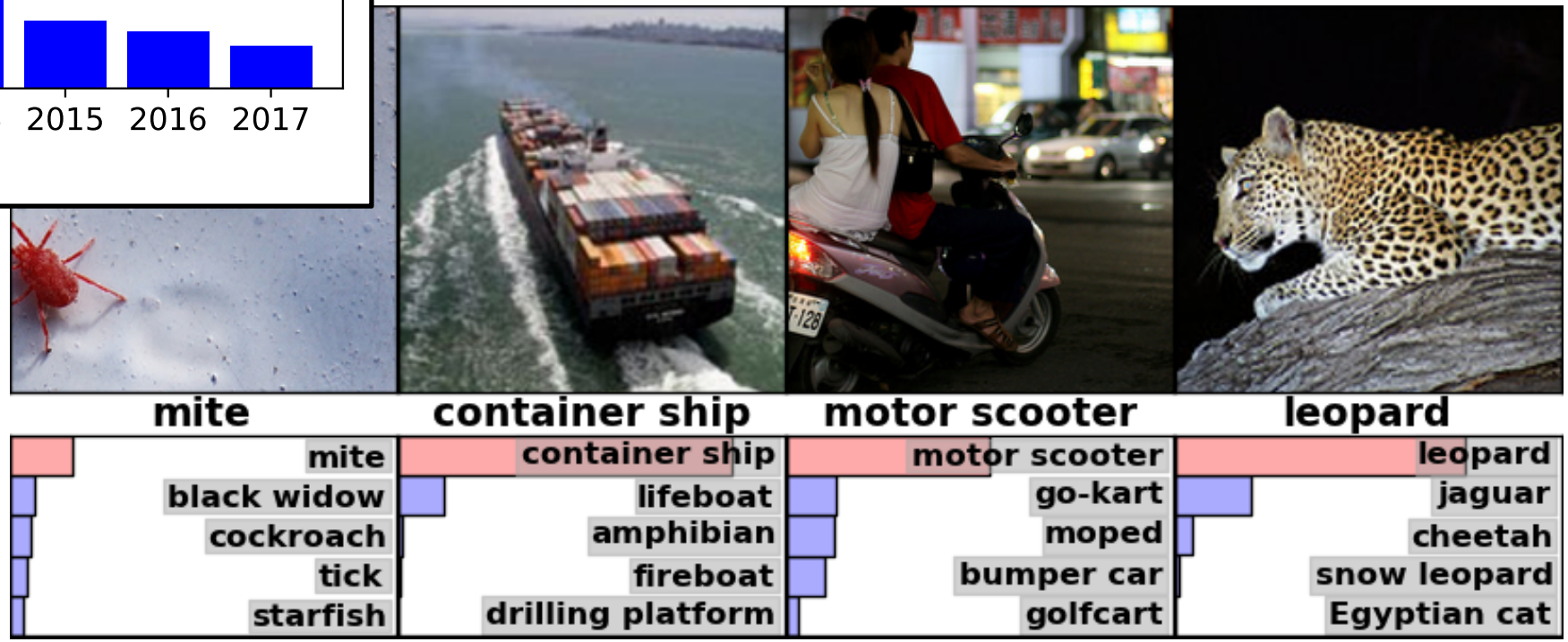
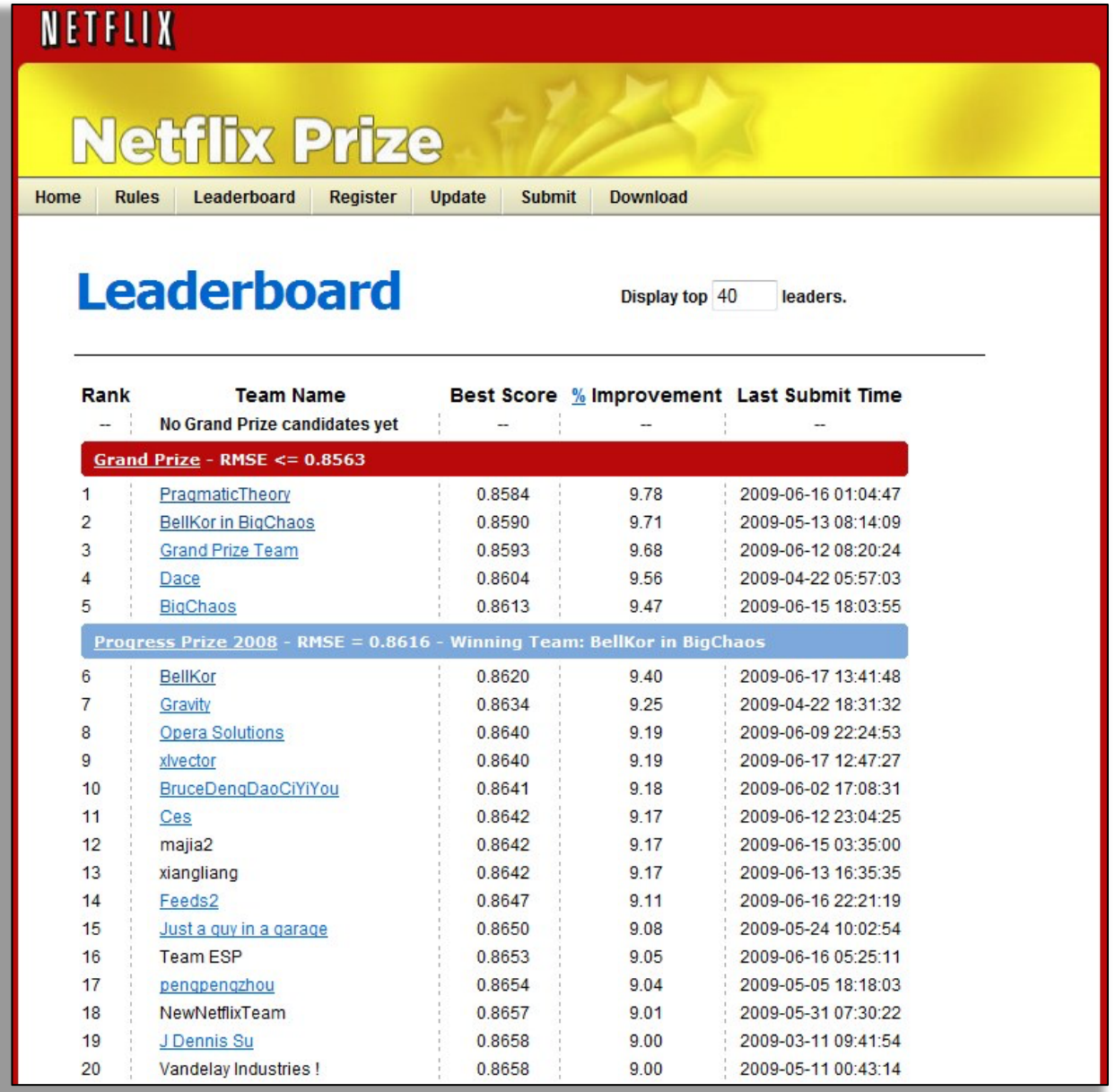
2016
2017
Year


mite
container ship
motor scooter
leopard
mite
black widow
cockroach
tick
starfish
container ship
lifeboat
amphibian
fireboat
drilling platform
motor scooter
go-kart
moped
bumper car
golfcart
leopard
jaguar
cheetah
snow leopard
Egyptian cat


NETFLIX
Netflix Prize
Home
Rules
Leaderboard
Register
Update
Submit
Download
Leaderboard
Display top 40 leaders.
Rank | Team Name | Best Score | % Improvement | Last Submit Time
-- | No Grand Prize candidates yet | -- | -- | --
Grand Prize - RMSE <= 0.8563
1 | PragmaticTheory | 0.8584 | 9.78 | 2009-06-16 01:04:47
2 | BellKor in BigChaos | 0.8590 | 9.71 | 2009-05-13 08:14:09
3 | Grand Prize Team | 0.8593 | 9.68 | 2009-06-12 08:20:24
4 | Dace | 0.8604 | 9.56 | 2009-04-22 05:57:03
5 | BigChaos | 0.8613 | 9.47 | 2009-06-15 18:03:55
Progress Prize 2008 - RMSE = 0.8616 - Winning Team: BellKor in BigChaos
6 | BellKor | 0.8620 | 9.40 | 2009-06-17 13:41:48
7 | Gravity | 0.8634 | 9.25 | 2009-04-22 18:31:32
8 | Opera Solutions | 0.8640 | 9.19 | 2009-06-09 22:24:53
9 | xlvector | 0.8640 | 9.19 | 2009-06-17 12:47:27
10 | BruceDengDaoCiYiYou | 0.8641 | 9.18 | 2009-06-02 17:08:31
11 | Ces | 0.8642 | 9.17 | 2009-06-12 23:04:25
12 | majia2 | 0.8642 | 9.17 | 2009-06-15 03:35:00
13 | xiangliang | 0.8642 | 9.17 | 2009-06-13 16:35:35
14 | Feeds2 | 0.8647 | 9.11 | 2009-06-16 22:21:19
15 | Just a guy in a garage | 0.8650 | 9.08 | 2009-05-24 10:02:54
16 | Team ESP | 0.8653 | 9.05 | 2009-06-16 05:25:11
17 | pengpengzhou | 0.8654 | 9.04 | 2009-05-05 18:18:03
18 | NewNetflixTeam | 0.8657 | 9.01 | 2009-05-31 07:30:22
19 | J Dennis Su | 0.8658 | 9.00 | 2009-03-11 09:41:54
20 | Vandelay Industries ! | 0.8658 | 9.00 | 2009-05-11 00:43:14

SHARE

SHARE

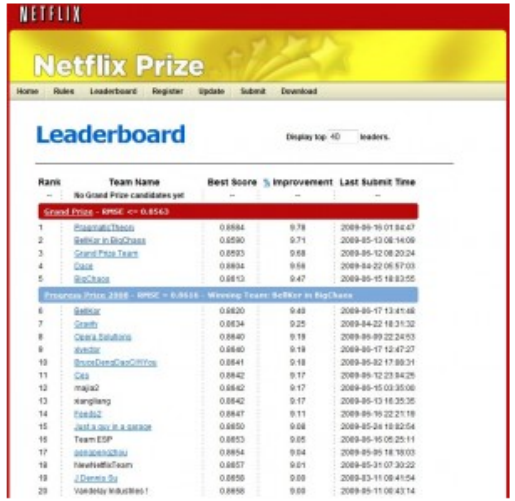
TWEET

COMMENT

EMAIL

CASEY JOHNSTON, ARS TECHNICA BUSINESS 04.16.12 08:20 AM

NETFLIX NEVER USED ITS $1 MILLION ALGORITHM DUE TO ENGINEERING COSTS



Netflix awarded a $1 million prize to a developer team in 2009 for an algorithm that increased the accuracy of the company's recommendation engine by 10 percent. But it doesn't use the million-dollar code, and has no plans to implement it in the future, Netflix announced on its blog Friday. The post goes on to explain why: a combination of too much engineering effort for the results, and a shift from movie recommendations to the "next level" of personalization caused by the transition of the business

Deep Learning is Approaching Human Performance in Language Understanding Tasks

Microorganisms or toxins that successfully enter an organism encounter the cells and mechanisms of the innate immune system. The innate response is usually triggered when microbes are identified by pattern recognition receptors, which recognize components that are conserve microorganisms, or when damaged, injur signals, many of which (but not all) are r those that recognize pathogens. Innate i meaning these systems respond to path not confer long-lasting immunity against is the dominant system of host defense

What part of the innate immune system identifies microbes and triggers immune response?

Ground Truth Answers: pattern recognition receptors | receptors | cells | tors

inant system of defense?

e system | innate immune

n

ize components present in broad

icroorganisms

in a generic way, meaning it is

non-specific | non-specific

Leaderboard

SQuAD2.0 tests the ability of a system to not only answer reading comprehension questions, but also abstain when presented with a question that cannot be answered based on the provided paragraph. How will your system compare to humans on this task?

Rank	Model	EM	F1
	Human Performance *Stanford University* (Rajpurkar & Jia et al. '18)	86.831	89.452
1 Mar 05, 2019	BERT + N-Gram Masking + Synthetic Self-Training (ensemble) *Google AI Language* https://github.com/google-research/bert	**86.673**	**89.147**
2 Mar 05, 2019	BERT + N-Gram Masking + Synthetic Self-Training (single model) *Google AI Language* https://github.com/google-research/bert	85.150	87.715


DeepMind
Workers: 14/16
AlphaStar
SC II HL


nature
THE INTERNATIONAL WEEKLY JOURNAL OF SCIENCE
At last — a computer program that can beat a champion Go player PAGE 484
ALL SYSTEMS GO

NO CHEATING!

You submit your model, and the organizers apply it to the test set, which is not publicly-available

Announcing the 2018 BHI & BSN Data Challenge

In collaboration with the IEEE Conference on Biomedical and Health Informatics (BHI) 2018 and the IEEE Conference on Body Sensor Networks (BSN), we are hosting a challenge to explore real clinical questions in critically ill patients using the MIMIC-III database. Participants in the challenge will be invited the present at the BHI & BSN Annual Conference in Las Vegas, USA (4-7 March 2018): https://bhi-bsn.embs.org/2018/

Will there be prizes?

Yes, prizes are sponsored by Google Cloud and Georgia Tech.

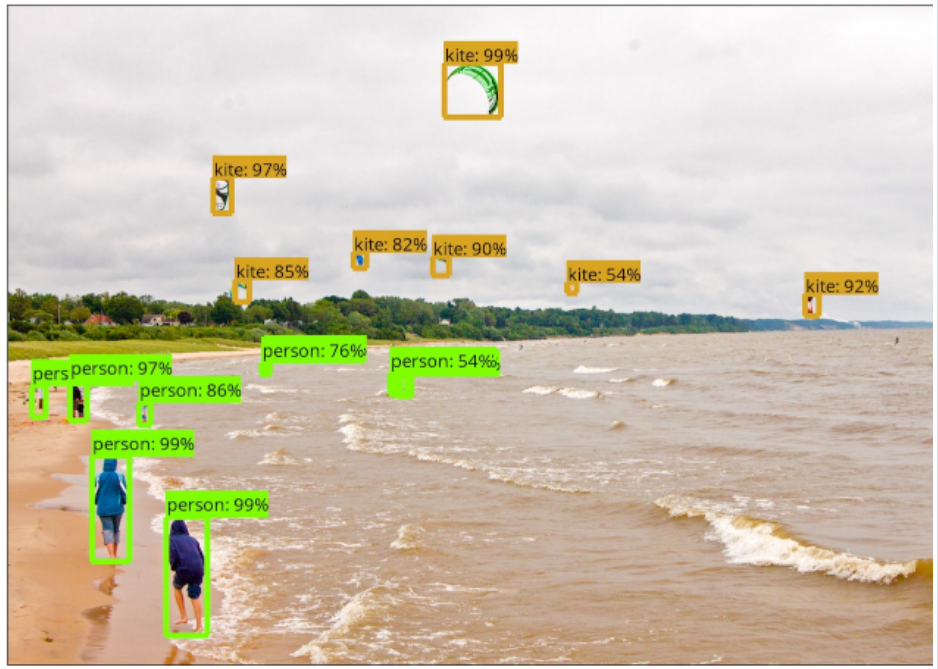
Google Cloud Georgia Tech

- Ingredient 1: Standardized evaluation of model performance
- Ingredient 2: Publicly-available training datasets
- Ingredient 3: Competition with Impartial Scoring
- Ingredient 4: Openness and code sharing

README.md

Tensorflow Object Detection API

Creating accurate machine learning models capable of localizing and identifying multiple objects in a sin
core challenge in computer vision. The TensorFlow Object Detection API is an open source framework bu
TensorFlow that makes it easy to construct, train and deploy object detection models. At Google we've c
codebase to be useful for our computer vision needs, and we hope that you will as well.



Contributions to the codebase are welcome and we would love to hear back from you if you find this AP
use the Tensorflow Object Detection API for a research publication, please consider citing:

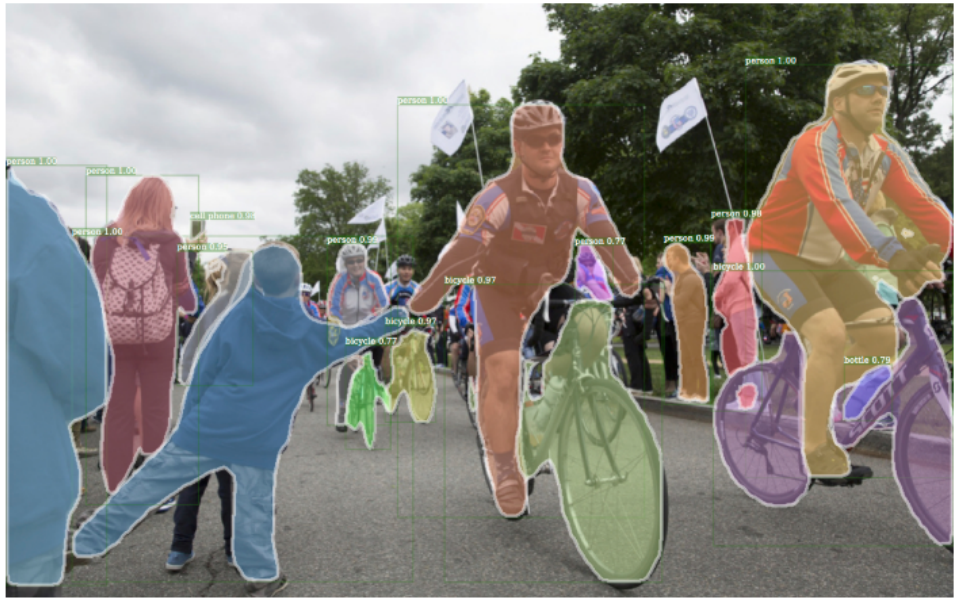
```
"Speed/accuracy trade-offs for modern convolutional object detectors."
Huang J, Rathod V, Sun C, Zhu M, Korattikara A, Fathi A, Fischer I, Wojna Z,
Song Y, Guadarrama S, Murphy K, CVPR 2017
```

README.md

Detectron

Detectron is Facebook AI Research's software system that implements state-of-the-art object detection algorithms, including Mask R-CNN. It is written in Python and powered by the Caffe2 deep learning framework.

At FAIR, Detectron has enabled numerous research projects, including: Feature Pyramid Networks for Object Detection, Mask R-CNN, Detecting and Recognizing Human-Object Interactions, Focal Loss for Dense Object Detection, Non-local Neural Networks, Learning to Segment Every Thing, Data Distillation: Towards Omni-Supervised Learning, DensePose: Dense Human Pose Estimation In The Wild, and Group Normalization.



Example Mask R-CNN output.

Less Stats Theory, More CS Theory and Culture

In 2001, William S. Cleveland (of Bell Labs) wrote that:

...[results in] data science should be judged by the extent to which they enable the analyst to learn from data... Tools that are used by the data analyst are of direct benefit. Theories that serve as a basis for developing tools are of indirect benefit.

He proposed 6 foci of activity, even suggesting allocations of effort.

- Multidisciplinary investigations (25%)
- Models and Methods for Data (20%)
- Computing with Data (15%)
- Pedagogy (15%)
- Tool Evaluation (5%)
- Theory (20%)

Several academic statistics departments that I know well could, at the time of Cleveland's publication, fit 100% of their activity into the 20% Cleveland allowed for Theory. Cleveland's paper was republished in 2014. I can't think of an academic department that devotes today 15% of its effort on pedagogy, or 15% on Computing with Data. I can think of several academic statistics departments that continue to fit essentially all their activity into the last category, Theory.

-- David Donoho, *50 years of Data Science*