# Lecture 11: ML Advice

Chris Ré

- This lecture is filled **with personal opinion** informed by building production, startups, clinical and research prototypes.
  - ***Biased with examples from my own work because I know it.***

- It is high level and presents some difficult, raw material.

- **Improve over time**: include ideas folks have told me were helpful to them.

- Will describe errors that I and collaborators have made or pointed out.
- **Goal is NOT** to cast aspersions but to get to better practice.
  - Many of these folks are my intellectual idols.
  - The worst errors are by far my own!

# Phases of ML projects

- Do you really want an ML system?
- Ok, so you want to train a model. It's not working well… now what?
- Now you have to live with an ML model and its eco system… yikes!

# A Running Example

- You want to build a spam detector.
- There are lots of types of spam, think of email for concreteness.

# 7 Steps of ML Systems.

# The 7 steps Overview

- Step 1: Acquire Data
- Step 2: Look at your data* -- after every step.
- Step 3: Create train/dev/test splits
- Step 4: Create/Refine a specification
- Step 5: Build model (simplest that works!)
- Step 6: Measurement
- Step 7: Repeat.

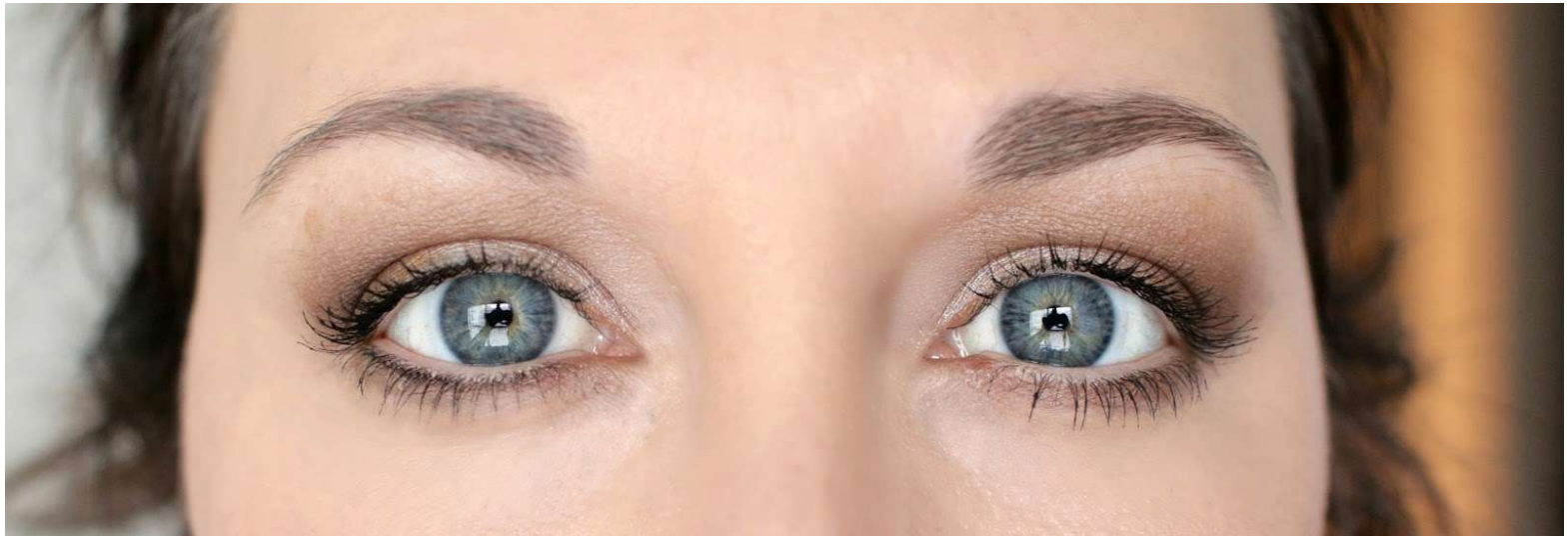
# Step 1: Acquire Data

# You need **realistic** spam (and not spam).

- Ideal data sampled from the data your SPAM product will be run on.
- Ideal not always available.
  - **Cold-start**. Feature doesn't exist yet!
  - Legal/ethical issues to look at data.
- You will get it wrong on 1st try.

# Data Artifacts are hard.

Any model may pick out **unintended signal.**
Modern, deep models may pick out ***more*** unintended signal.



Kuehlkamp et al. *Gender-from-Iris or Gender from-Mascara*

**Upshot**:
Picked up on
*mascara*

Hidden data artifacts are very challenging!

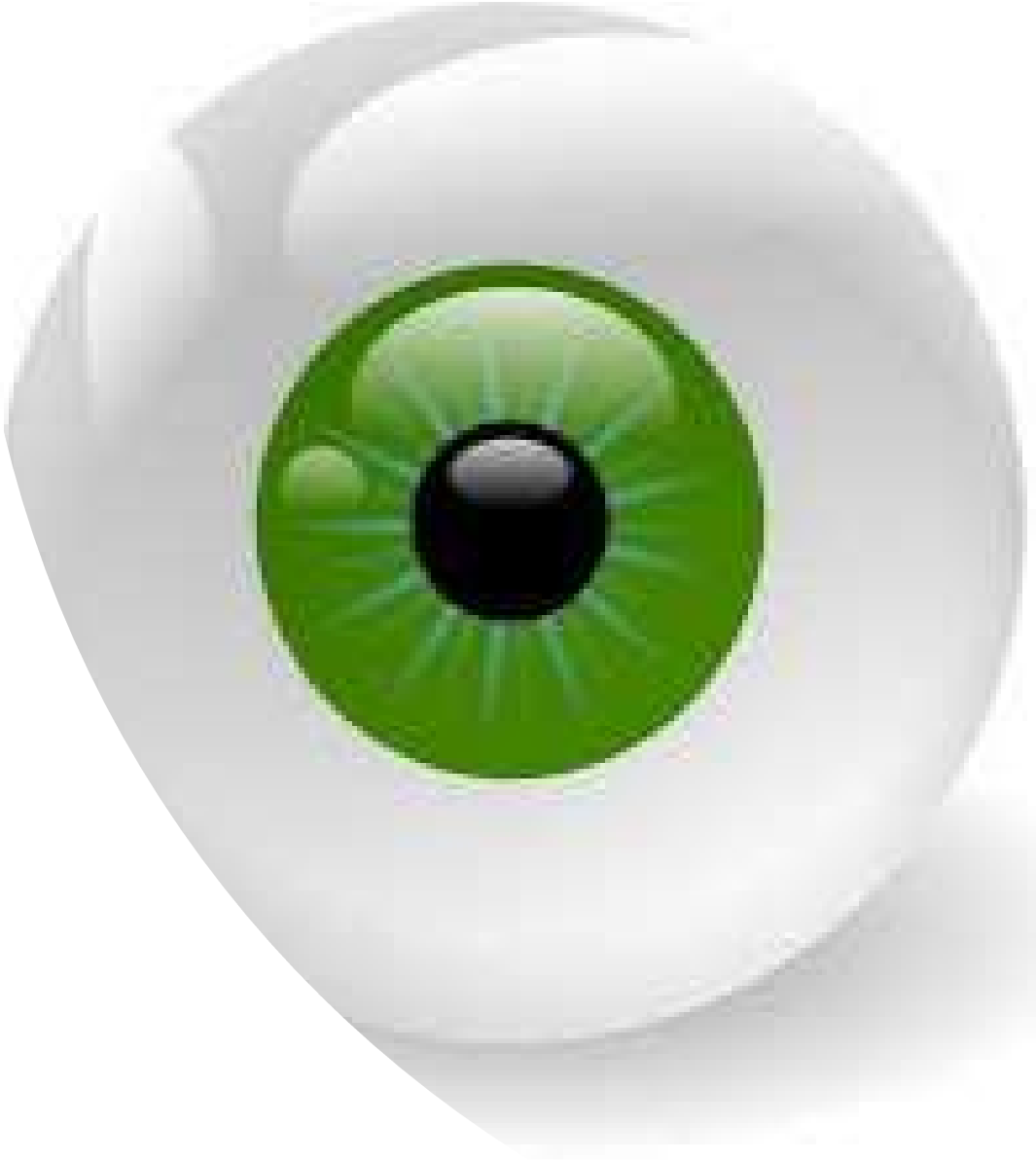
# Step 2: Look at the data

# Look at your data.

- You have some spam, look it at it!
- If needed, build tools to look at your data.
  - Spam from Europe different than from Africa? from US?
  - Spam to .edu different than .com?

- “Become one with the data” – Karpathy.

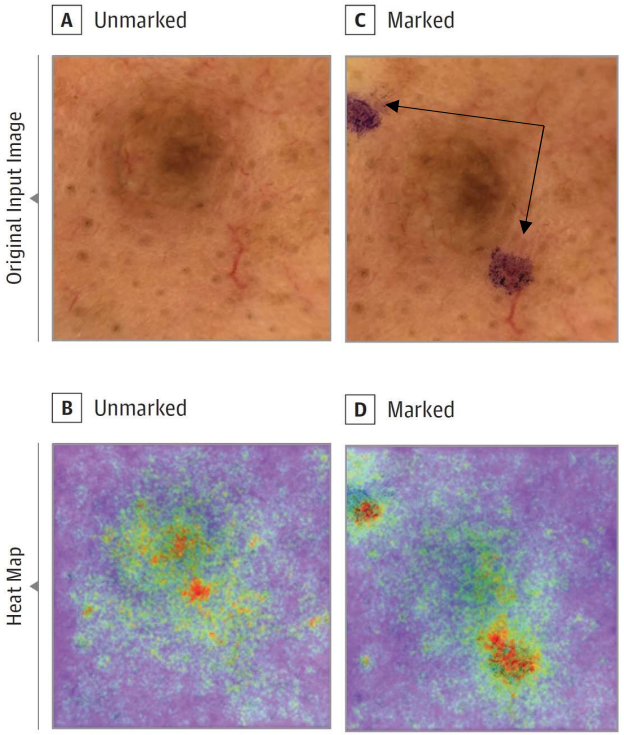
- Do this at every stage!



Have the **right people** look at your data

# Expertise is often required!

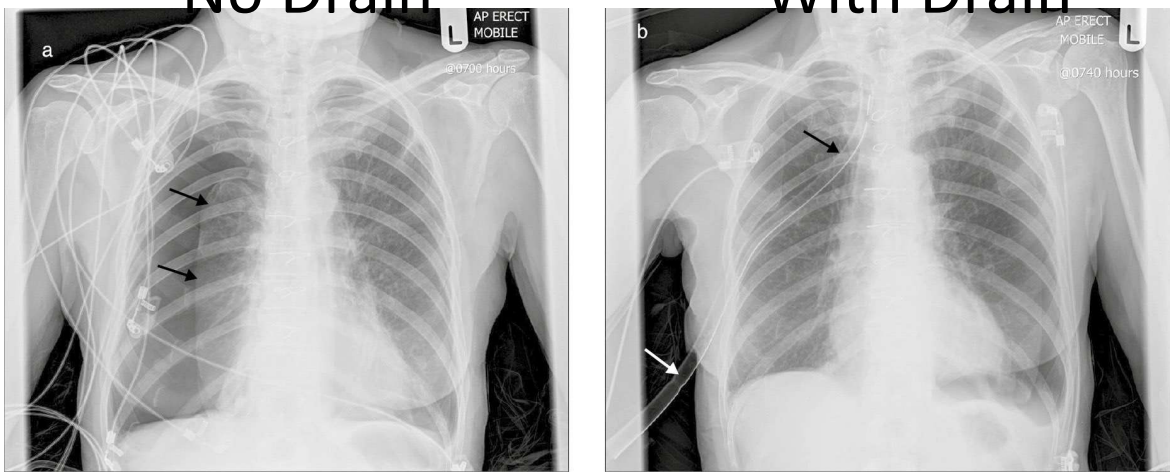
## Melanoma Recognition (Surgical Marks)




## Pneumonia Detection (Chest Drains)

No Drain

With Drain




Pneuomthorax has 0.94 AUC—with chest drains—but 0.77 without… ***Chest drain means already treated!***


Image Credits

Valchanov, Kamen, Nicola Jones, and Charles W. Hogue, eds. *Core Topics in Cardiothoracic Critical Care*. Cambridge University Press, 2018.

Winkler, Julia K., et al. "Association between surgical skin markings in dermoscopic images and diagnostic performance of a deep learning convolutional neural network for melanoma recognition." *JAMA dermatology* (2019).

https://lukeoakdenrayner.wordpress.com/2019/10/14/improving-medical-ai-safety-by-addressing-hidden-stratification/

# For more detail see…

Gustavo Carneiro (Adelaide)

Luke Oakden-Rayner (Adelaide)

Jared Dunnmon (Stanford)

**Hidden Stratification Causes Clinically Meaningful Failures in Machine Learning for Medical Imaging**

# Step 3: Train/Dev/Test Split

# Partitioning Data: Train, Test, and Validation

(1) Fit model to the training dataset

(2) Fit hyperparameters to the *validation* (or *development*) dataset

(3) Test model performance on the test set

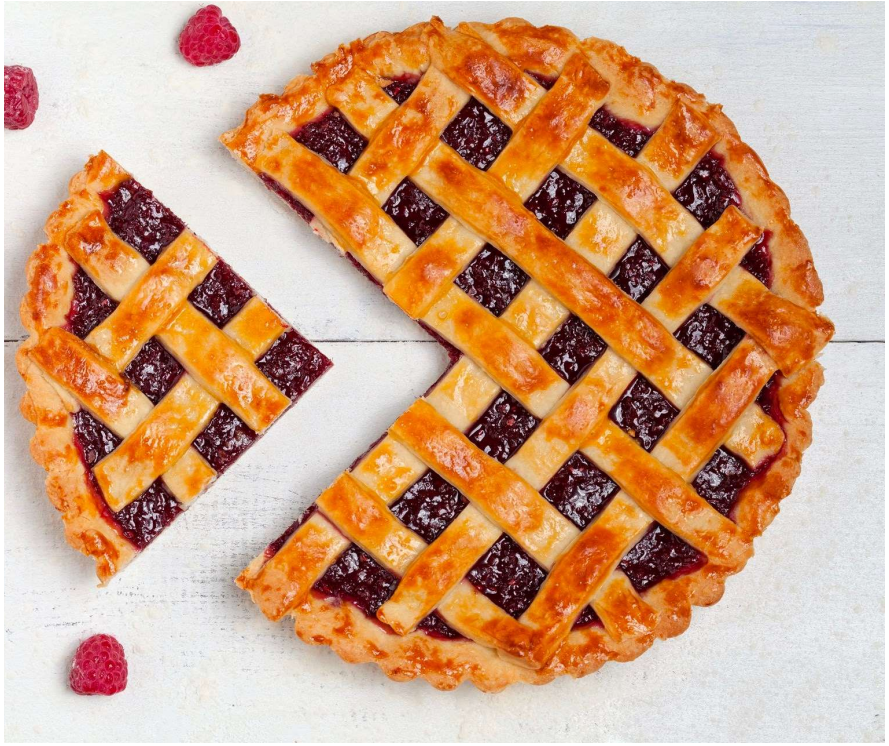
Critical to avoid leakage / adaptive overfitting

# What makes a good split?

- **Ideal**: Train, test, & dev randomly sampled
  - Allows us to say train quality is approximately test quality.

- But, test is a **proxy** for the real world!
  - We'll talk more about this later…

- **Challenge**: Leakage.
  - (Nearly) same example in train and dev.
  - Causes performance to be overstated!
    - Eg., same senders in train and test?



# Random isn't the only goal.

**Given:** 50 company stock price for 100 days

- Triples of the form (Company, day, price.)

**Goal**: predict stock prices (Ahead of time for $)

What happens if you **randomly** split into halves?

- Train contains { (GOOG, day 10, 126), (GOOG, day 12, 1275) }
- Test contains { (GOOG, day 11, 1270) }

**Better split**: Use first 50 days to predict last 50 days?

- More later…

***Our split doesn't reflect our predictive goal!***

# Step 4: Create a specification

# Create a specification

- Machine learning doesn't obviate the need to know what you are building.
  - What is SPAM? Maybe I like ads for low low rates?
- A good specification has little ambiguity.
  - What level of expertise is required to understand it?
- Your specification **must** be embodied in **a set of examples. A test set!**

# Quick and Dirty Test: Inner Annotator Agreement

- You write down your notion of SPAM. Select N randomly selected examples. Give to three different annotators.
  - **Inter-annotator agreement.** How often do annotators agree?
- Let's say annotators agree 95% of the time—great!
  - **The meaningless accuracy problem.** *Can you build a product with greater than 95% accuracy against this spec?*
- Examine the spec & disagreement cases.
  - Train annotators or change spec?
  - If a humans can't agree, the machine is going to have trouble…
- Do you train the people or the machine? (serious Q)

# Subtle Problem: *Consistency in test sets*

**Consider following protocol.**

- Every day, sample data
- Send examples to crowd
- Get grades back

# Subtle Problem: Spec creep

- **Warning:** Tempted when answer is *"pretty good"* to say yes–for classification this must be precise or you accrue rot.
  - **Label rot—not debt** hard to find once there! You should clean it up!

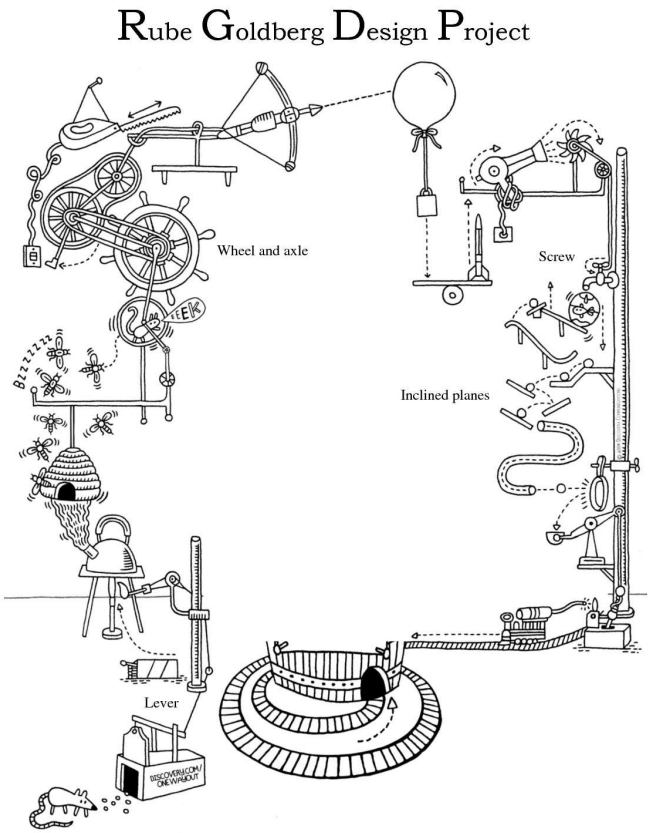
- **Spec**: Unsolicited drug ads should be marked drug spam.
- Spam for vitamins comes in—and is successfully filtered.
  - This answer is marked as drugs and filtered.
  - Answer is useful, but allowing it may cause **scope creep** (are vitamins drugs?)
  - If you yes, revise the specification!

# Step 5: Implement simplest possible model

# Keep it simple!

- If python code can get 90% accuracy, use it!
- If python code can get 100% accuracy, use it!
- ML shines on a class of problems:
  - can be **precisely specified** but
  - Writing down program is prohibitively hard

- **Avoid getting bogged down in *<u>new</u>* models, use them to understand the data!**
  - Models can be tools (scaffolding), not just end goal.



# Value of Baselines

- Someone will ask if your change is worth it, **be prepared**.
  - If your fancy engine buys 0.1% but runs 1000x more slowly… or needs 1000x more data…

- *Build simpler methods **even after** fancy models.* Often use deep models to *"come up with features"* – by looking at output!
  - Models can be a tool to understand data!

# Ablation studies.

- You’ve built up a model, it has many different components.
  - Which matter?
  - which are stable?
- Remove one feature at a time!
  - *Adding* features + baseline could overestimate overlap. How?
- Measure performance.
  - Critical for research!

Step 6: Measure the output!

# Simple descriptive dashboards

- **Challenge**: Don’t make the same mistake twice!
  - Measure end-to-end quality metrics.

- **Challenge**: catch new mistakes, asap.
  - Harder!
  - Measure simple things
    - How many entities per sentence? How long are the sentences? How many verbs? Keywords per sentence.
    - Slice by time. Is your SPAM changing over time?

# Avoid Known mistakes Slice-based Monitoring.

- Overall performance may not be as critical as important “slice”.
  - “Call mom” should work
  - More complex queries may be less expected.
- Record & scoreboard on these slices.
- Your monitoring should have support for fine-grained reporting!

# Robustness Gym

## Research and Tools

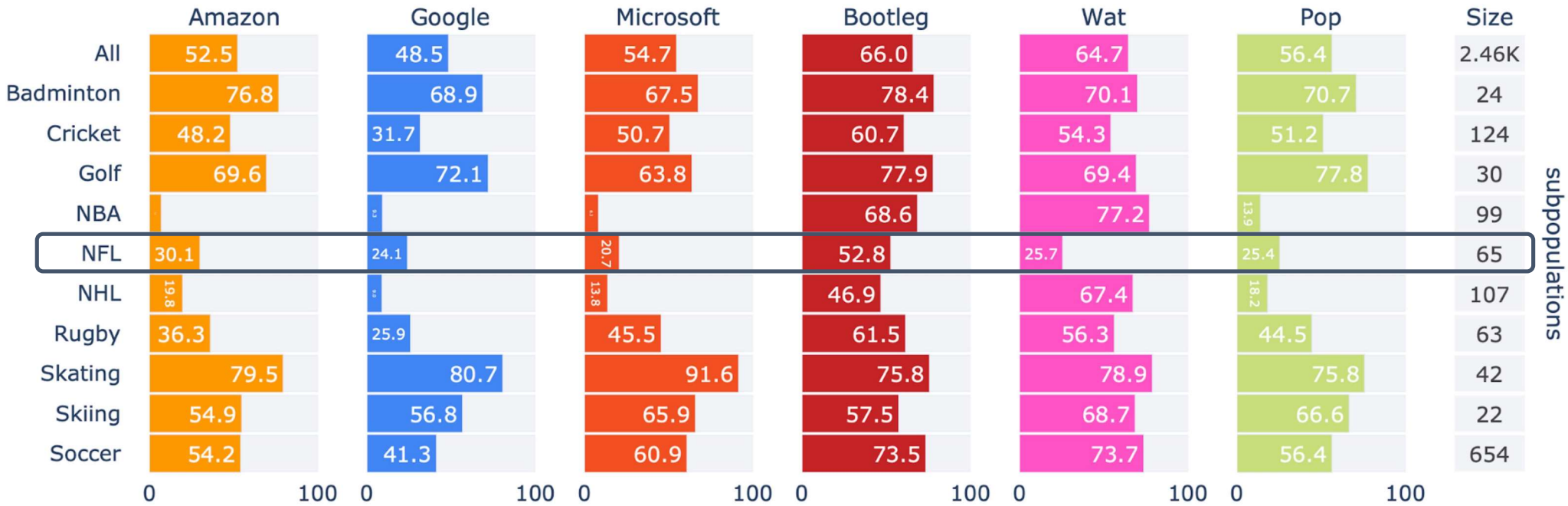
fine-grained model evaluation, analysis and beyond!

Stanford University

salesforce

UNC NLP

# All Systems Make Mistakes




F1 Scores on NED

CoNLL AIDA

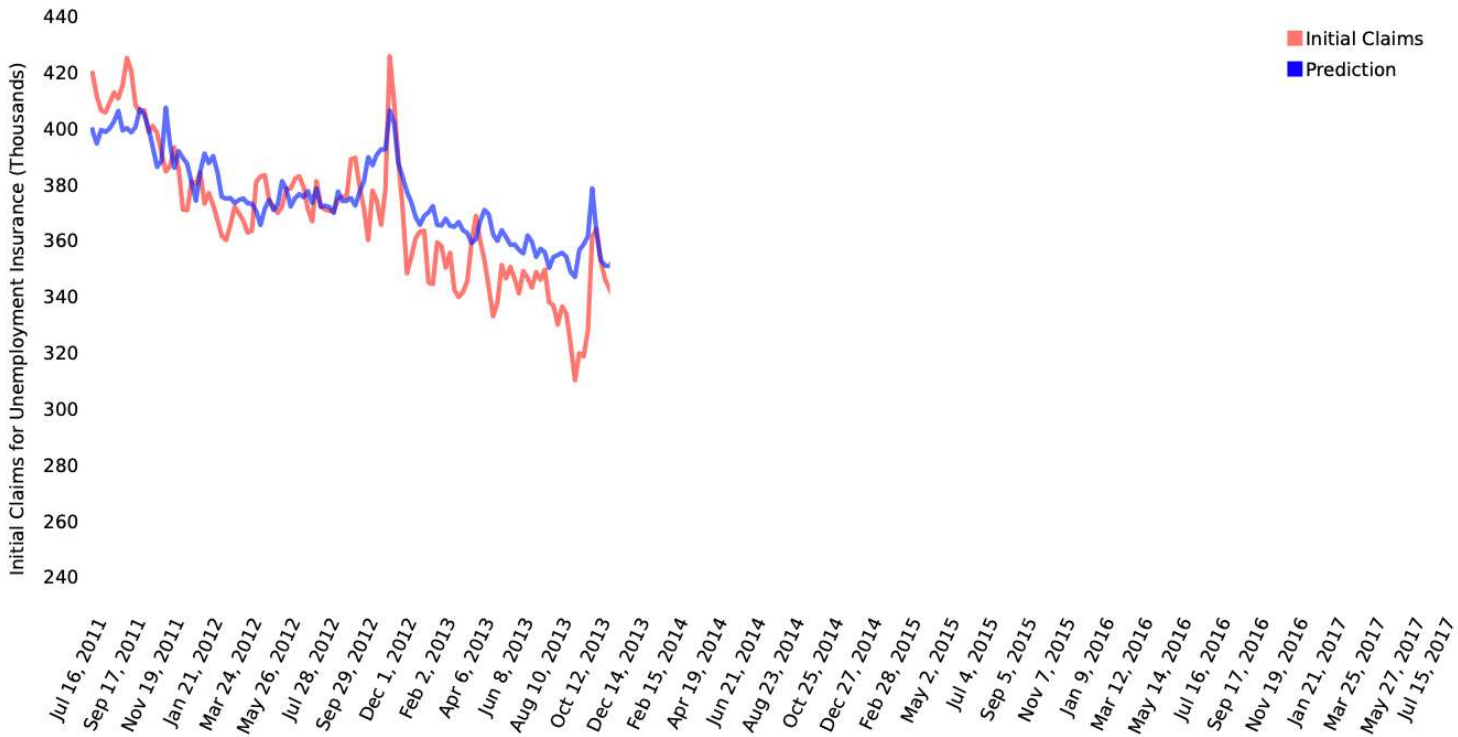
# Challenge: Avoid *unknown* mistakes

- Distribution shift is a real issue.
  - **Popularity Shift/Cold-start.**
    - You release a feature, queries that weren't popular are now **very popular.**
    - Old score says "we're great", but felt experience is awful.
    - **Remedy**: Hopefully, you knew this slice was coming and you monitored it proactively.
  - **Input Shift.** Your input changes in some way.
    - Much harder to catch in my experience…
    - More next!

This is incredibly hard! No ideal solutions in industry...

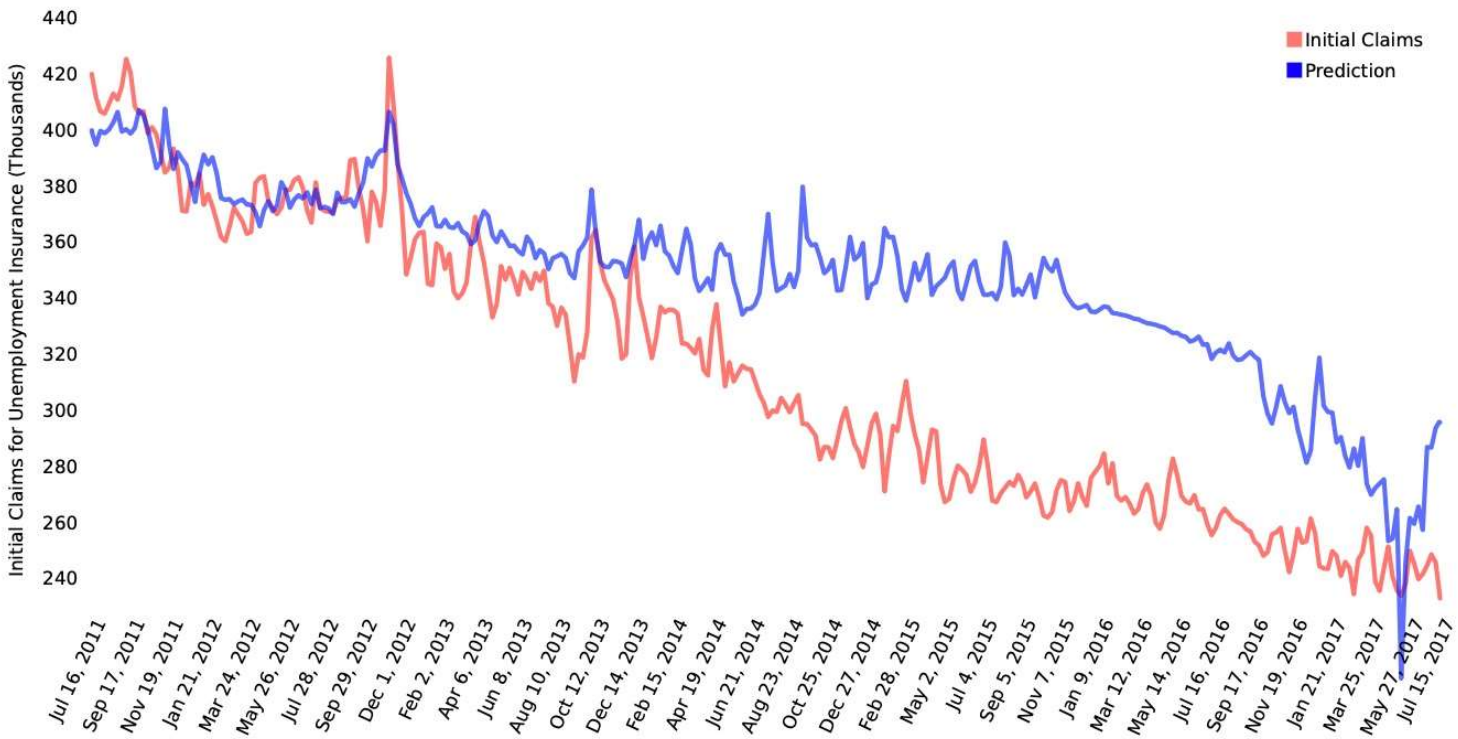
*I've gotten this **very** wrong…*

# Predicting unemployment claims from Twitter (at time of publication)




Courtesy: Keith Winstein

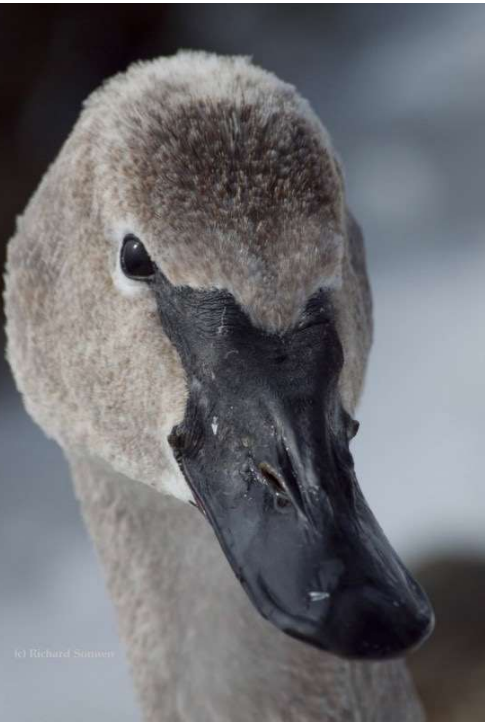
# Predicting unemployment claims from Twitter (post-publication)




What went wrong?!?

Courtesy: Keith Winstein

# Postmortem:
# Three identified issues—many remain!

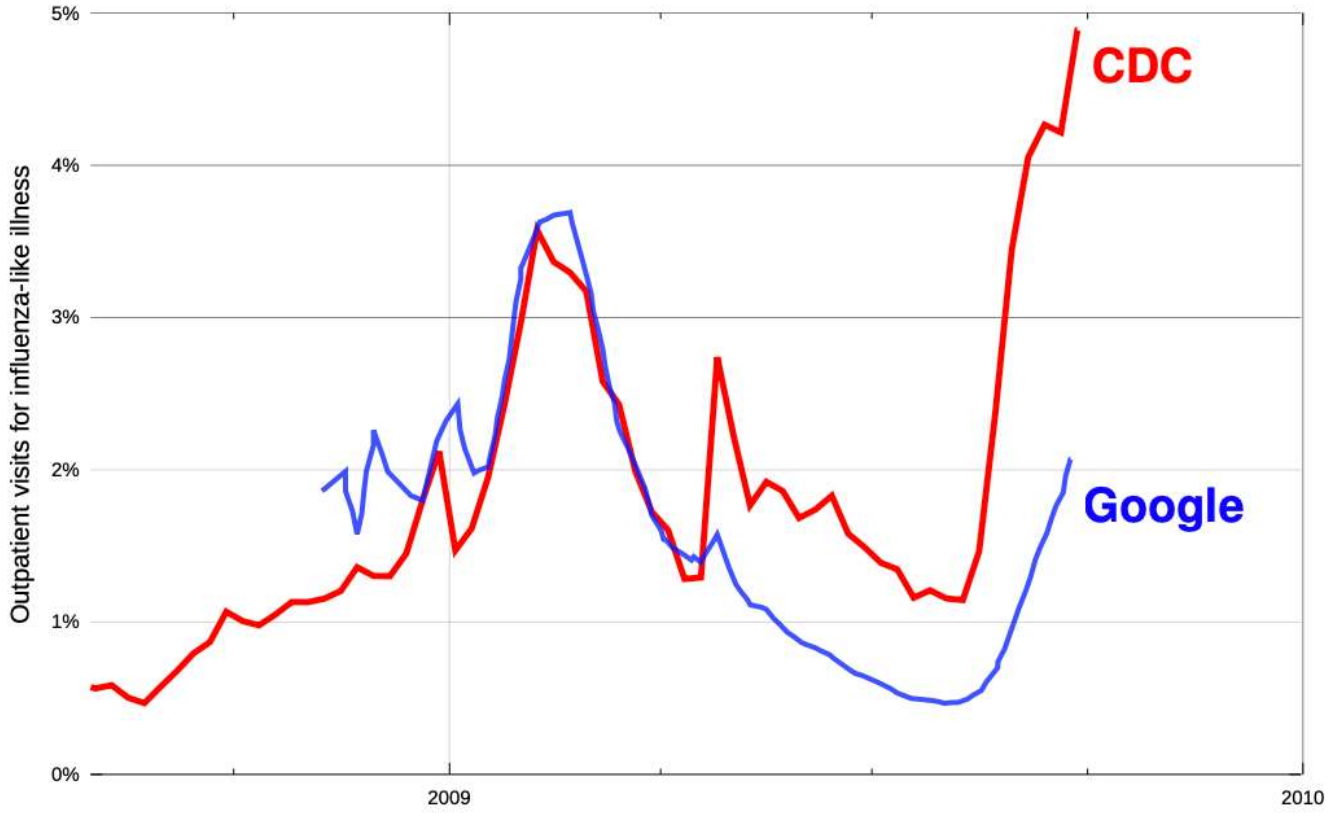


- Twitter changed the text filtering model reflecting business priorities.
  - This is **common** in most systems! How do we control for it?
  - *Cope retraining—we imperfectly understand substrate and it can change!*
- Model sensitive to outliers ***"Gray swans"***
  - Mined keywords like *"pink slip"* were used as part of an advertising campaign.
  - *Median regularization to deal with feature spikes.*
- Economic reality changed in 2014
  - Losing a job meant you quickly got a new job—stale more quickly.
  - *Used PCA to help diagnose changes…*

http://web.eecs.umich.edu/~michjc/cafarella-nas-census.pptx

Courtesy: Keith Winstein

## Performance in the first year




http://blog.keithw.org/2013/02/q-how-accurate-is-google-flu-trends.html

# Labels & Input Drift (change) over time.

Automatic monitoring matters.

Adapting to customer taste change.

This is **REALLY** hard

# Step 7: Repeat! (And Look at your data!)

# The 7 steps recap

- Step 1: Acquire Data
- Step 2: Look at your data* -- after every step.
- Step 3: Create train/dev/test splits
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- Step 5: Build model (simplest that works!)
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I have yet to see anyone get preceding steps right on first try. *Build quickly and iterate.*

*A well running ML system is a*
***rewritten** poorly running ML system.*

# More detailed version

- Specification Challenges
- Model Training and Performance Diagnostics
- Monitoring Challenges
- Issues in Shipping to Production/Use

# Specification

# Types of Errors in Specification

- Class schema issues
  - Two distinguishable classes merged as one
  - One class split into two now indistinguishable class
- Unknowable class.
  - Information to distinguish two different cases is not available to the model
  - More common than you would think!
- Unrealized structure between classes
  - For example, fine-grained errors may not count as much as coarse-grained errors.
- Test set label variance
  - If this (e.g. inter-annotator disagreement) is > the error deltas being tested for, nonsensical!
- Change between test set versions
  - Test sets need to be regularly “refreshed”- need to watch for changes between versions!
  - More later…

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# Class Confusion Matrices

| | Class LoanSpam | Class Phishing | Class Good Email |
|---|---|---|---|
| **Predicts LoanSpam** | 1000 | 10 | 50 |
| **Predicts Phishing** | 45 | 505 | 30 |
| **Predicts Good Email** | 7 | 8 | 2000 |

- See at a glance, our accuracy is pretty high (look at diagonal)—but…
  - Discuss our false positive v. false negative rates?

- What would happen if we added spear phishing? Can help us debug specification!
  - Examine "top confused classes" if you have many
  - Common when building big ML models collaboratively. (duplicate names for a concept)
  - Subtle distinctions are good!
    - **Crisp.** If they manifest differently in data and we can define this difference.
    - AND we have enough data.

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# Spoiler: It's a pipe.
# *(Your Ground Truth Contains Errors)*

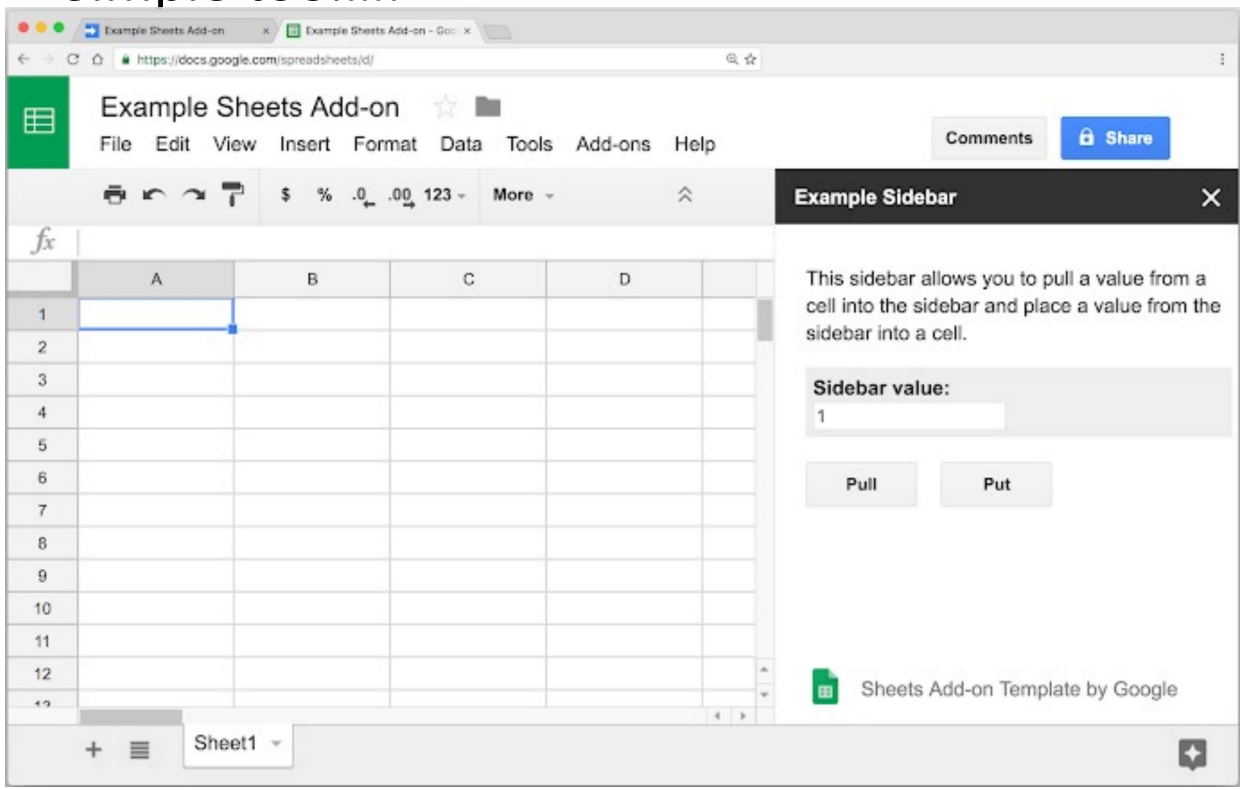
- **"ground truth"** is constructed.
  - Fix the specification..
  - Fix the data
  - *It is a curated resource!*

- ***Measure Error!*** *If your error rate in GT is 3%, then 1% change may not be meaningful.*

"This is not a pipe."

# Look at the data! Nothing fancy.

- Simple tool….



Labeling party!

# The art of errors

- Split the error buckets into buckets such that there is some **systematic** information the model is missing.

- A good bucket for “relationship extraction”
  - “Her husband, Barack Obama,…”
  - “Her sister, Venus Williams…”
  - “His wife, Serena Williams…”
  - Aha! Missing “relationship name and appositive”
- It’s an art, if you can’t group buckets—you may be tapped out!
  - Convert high-level insight into features is an art and skill—practice it!

# Selecting more labels

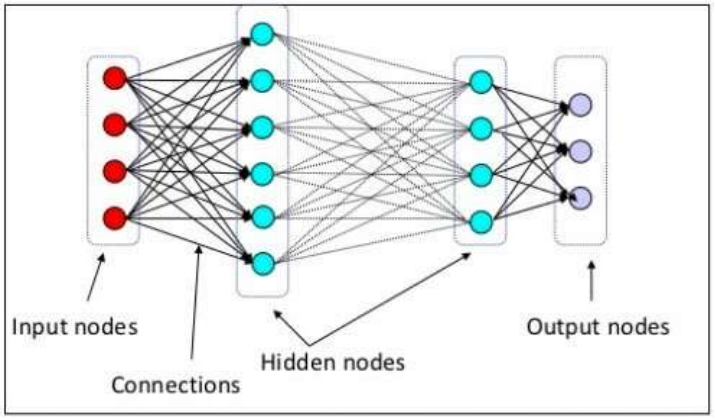
- It's all about sampling!

- Uniform Random Sampling (URS)
  - Advantage, you'll improve the **overall** error
  - Statistically safe.

- Importance-based sampling.
  - Can be cost effective—if your class only appears 1 of 10k times, would be expensive to use (URS)!
  - Pick near misses? *"more informative"*
  - *Don't use for evaluation by itself. Why?*

# Error Analysis in the Era of Deep Learning

- Error bucketing is **still critical**.
- **Minor miracle**: often, you can add labels to drive model to predict the right class!
- Selecting the *right examples* is important.



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# Do CIFAR-10 Classifiers Generalize to CIFAR-10?

Benjamin Recht
UC Berkeley

Rebecca Roelofs
UC Berkeley

Ludwig Schmidt
MIT

Vaishaal Shankar
UC Berkeley

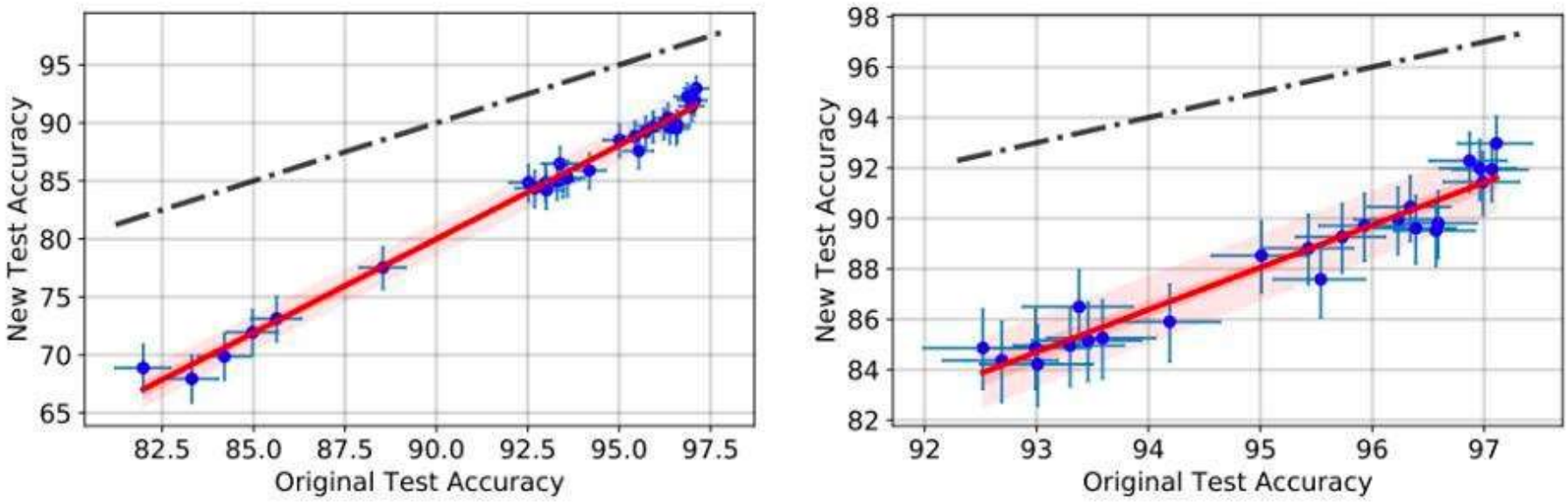
June 4, 2018

# Do ImageNet Classifiers Generalize to ImageNet?

What if we sampled a new test set according
to the same specification as the original?

*Expect the same outcome!*

# No real evidence of adaptive overfitting!



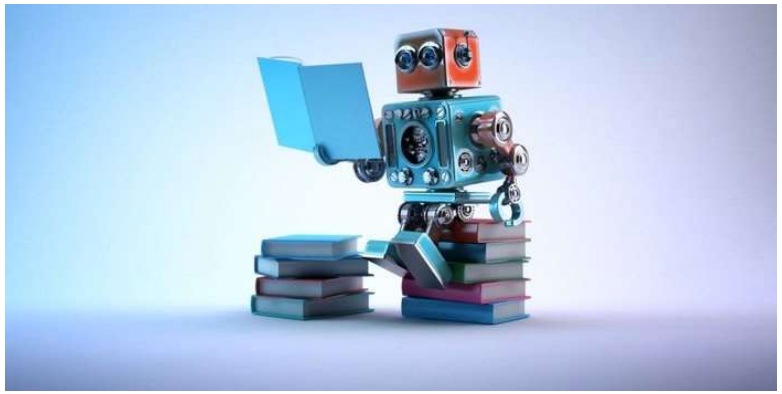

(a) All models

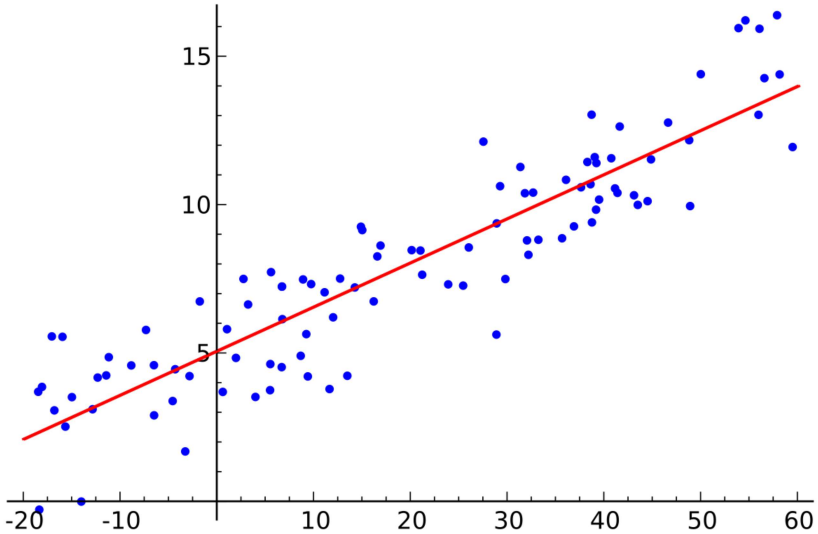
(b) High accuracy models

But specification and distribution shift hit you! Same on ImageNet

# Model Diagnostics

# You want to build an ML model






## Which should you build first?

*…try simple methods first… really still debugging.*
*Best ML folks treat models as a way to understand.*

# What to build?

- Build simplest thing first.
  - Sometimes what you have code/model laying around… iterate quickly!

- Linear or logistic regression w/ simple features,
  - You know it’s converging, easy to setup, lots of packages that support it.
  - It runs fast! Quick iteration!
  - Features are easier to understand, add information, do error analysis.
  - Good baselines for future work
  - Many projects get good enough results here, and move on.
  - Or, more often, learn that they didn’t understand the problem and refine!

# Debugging Learning Algorithms

- Your goal is to build an ad spam detector.
- You run a logistic regression algorithm.
- Sadly, it's error is too high!
- What do you do?

# What could be wrong?

- Maybe it’s the data or your features?
  - Try getting more training data.
  - Try a smaller set of features?
  - Try adding more features?
- Maybe it’s the optimization algorithm?
  - Run GD a little while longer….
  - Try a different method, SGD, GD, Newton?
- Maybe it’s the hyperparameters?
  - Different value of regularizer?
- Try using a different model!

**if you don't tell me what's wrong, how can i make it right?'**

# Just like compiling!

- Could hit train model, try it, and run again!
- Or you could develop **diagnostics to help you understand.**

- Recall simple metrics, these catch **data prep bugs (very nasty)**
- Bias-variance provides a set of diagnostics!

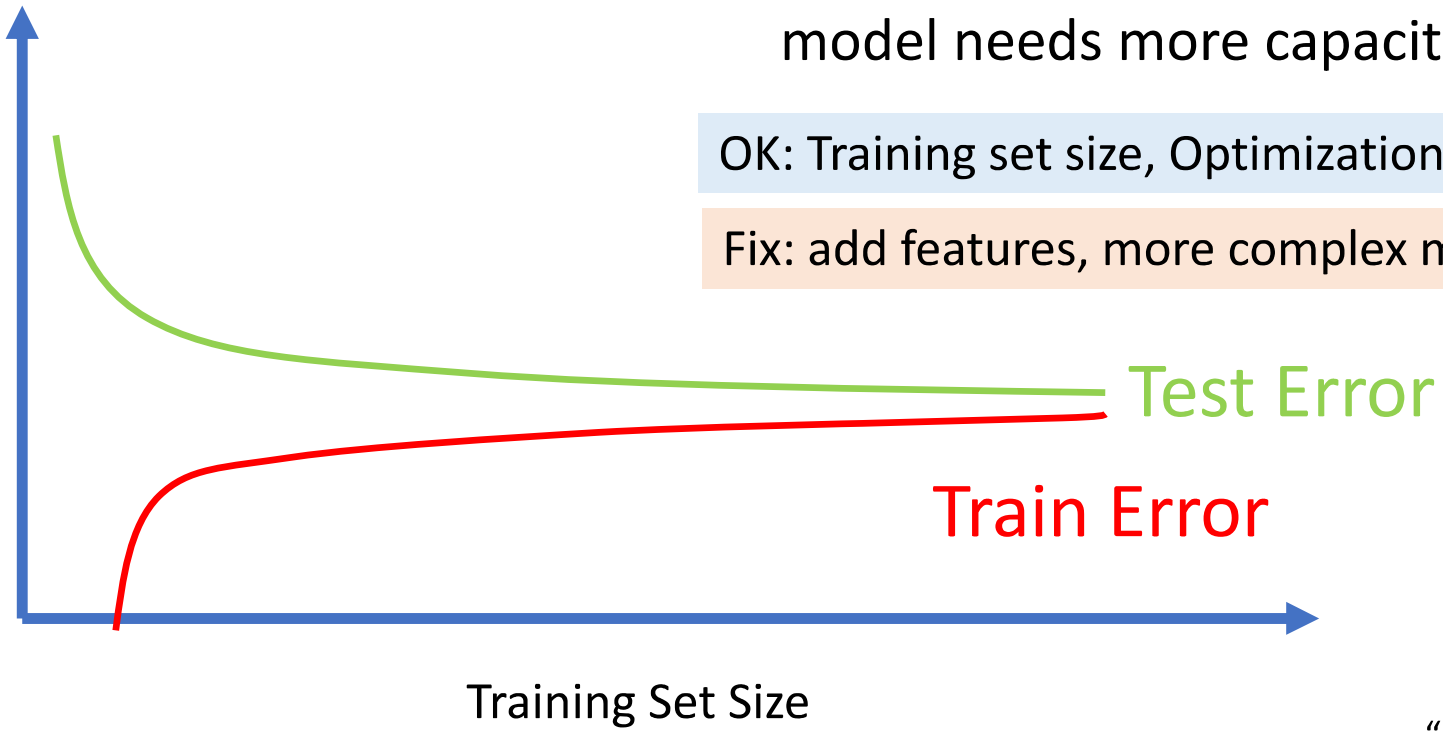
We'll cover some diagnostics that have helped us.

# Diagnostic: Test versus Train Score.

*If error is too high*:
model needs more capacity!

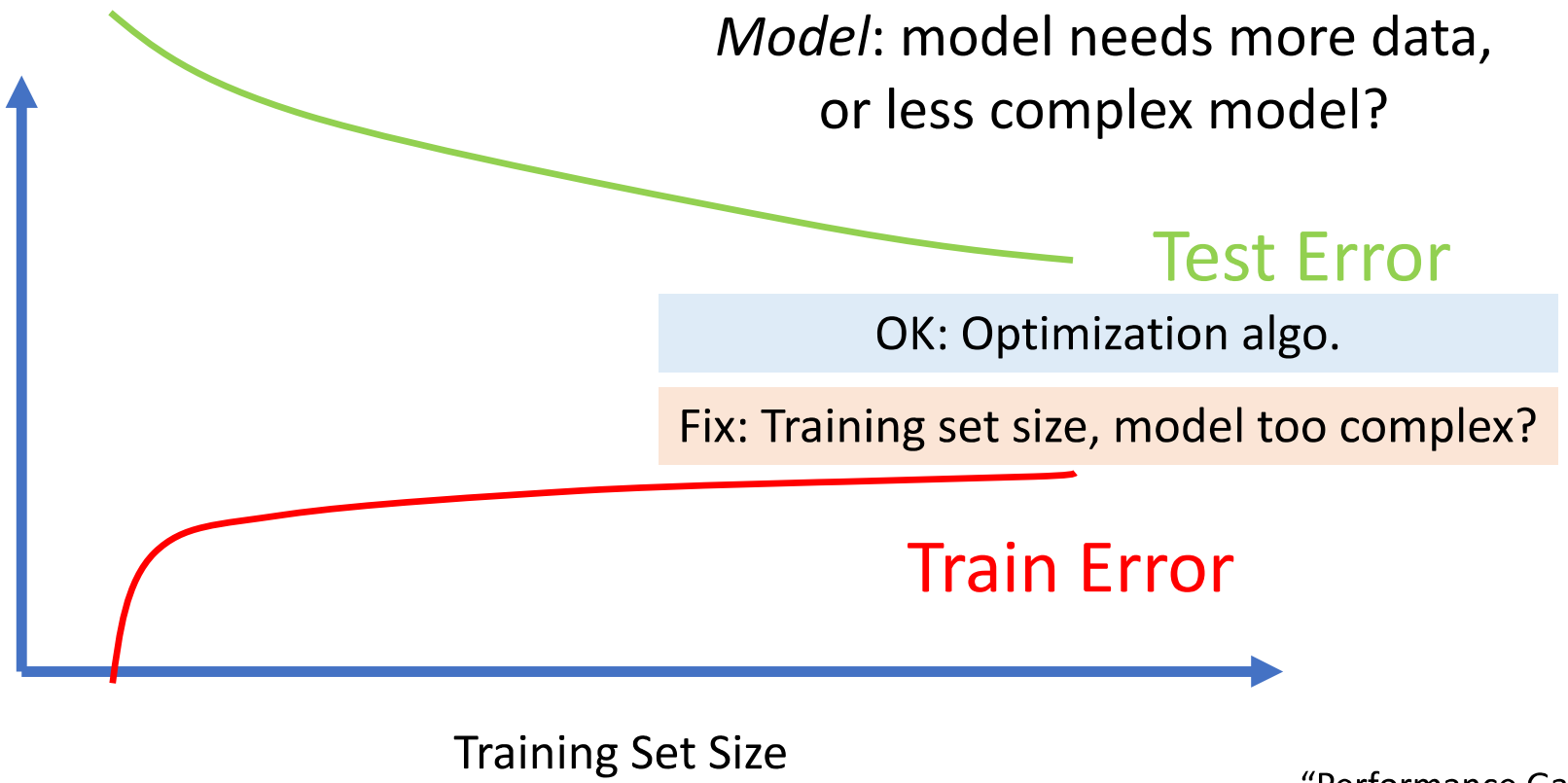
OK: Training set size, Optimization algo.

Fix: add features, more complex model




"Test=Train"

# Diagnostic: Test versus Train Score.




"Performance Gap"

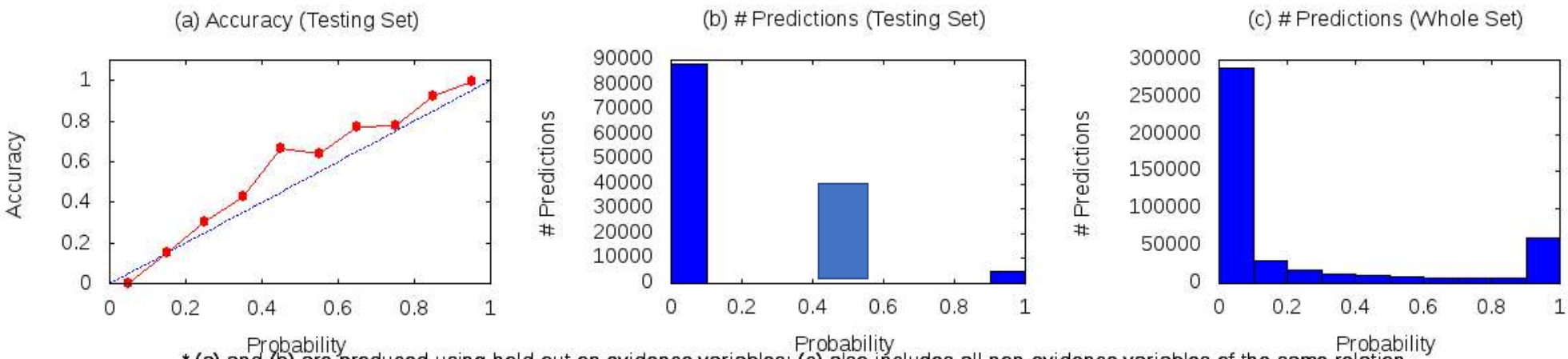
# Variance Diagnostic

- Variance diagnostics.
  - Sample data set (k-fold cross validation)
  - Train on different folds.

- If the dev scores diff are small relative to your target error, you're OK!
  - If you're target error is 10%, and your variance ~ 1% fixing variance doesn't matter!
- If larger, too little data or algo. instability!

# Diagnostic: Calibration Plots!

- Your spam detector uses logistic regression (or softmax last layer)




* (a) and (b) are produced using hold-out on evidence variables; (c) also includes all non-evidence variables of the same relation.

It's calibrated.

This bump means there is a lurking class!
Need more features. "Calibration Bump"

# What could be wrong?

- Maybe it's the data or your features?
  - Try getting more training data.
  - Try a smaller set of features?
  - Try adding more features?
- Maybe it's the hyperparameters?
  - Different value of regularizer?
- Try using a different model!

Performance Gap

Performance Gap

Train = Test, Calibration bump

# Really rough guidance

- If your test error is OK, good for now!

- Else, if train == test
  - Fix: you need a more complex model.
- If train < test you're overfitting.
  - Fix: Regularize, less complex model

- If train oscillates wildly, you have a problem with your optimization algorithm.

- If train goes down lower with method A than method B, then prefer method A ☺

# They're all just weights.

- Train another model on the same features.
  - SVM, logistic, even linear—as long as
- Suppose new model does better but you want to use the old model!
- You can plug in your new model into your old objective.
  - If loss is lower → optimization problem!
  - If loss is higher -> model problem. (harder)
  - Examine where they differ can reveal capacity differences.

# Diagnostics Summary

- Some I've used or seen teams use well.
- Cleverness to come up with your own.
- Think "unit testing". It's engineering.

# Advanced Techniques and Recent Studies

# Selecting features

- You derived some of the L1 technique (Lasso).
- Recall: Selects a sparse model weights..

- It enables you to select models, this changes how you build the models—often toss in many features, let it pick!

- You can freeze known good features, select among new features.

https://scikit-learn.org/stable/auto_examples/linear_model/plot_lasso_lars.html

http://statweb.stanford.edu/~tibs/ftp/lars.pdf

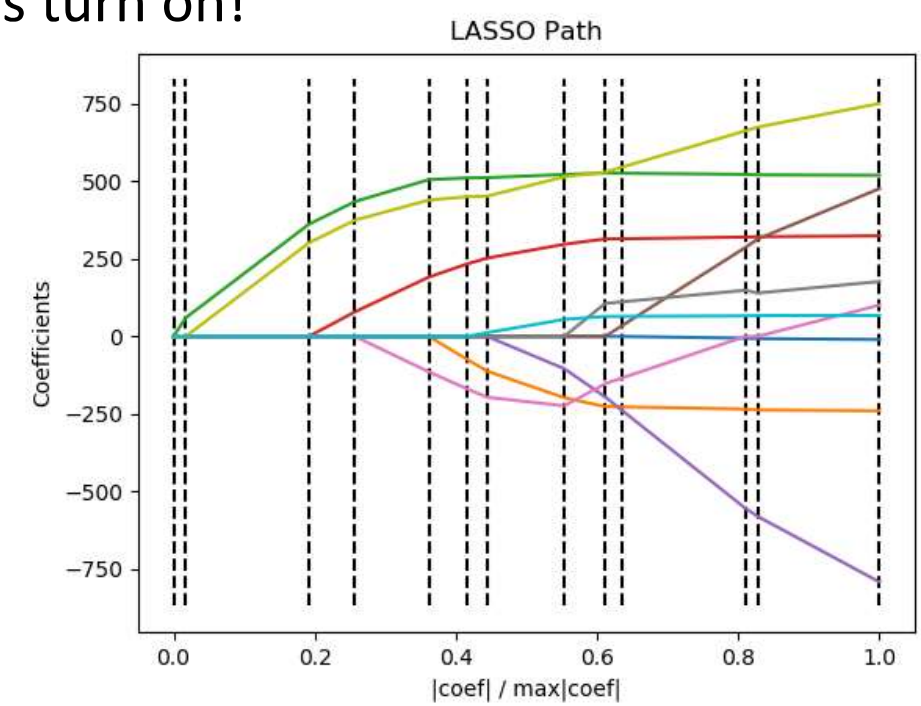
# Lasso Path

Main idea: Sweep the regularize parameter for L1, train the model, see when features turn on!

**LEAST ANGLE REGRESSION**

BY BRADLEY EFRON,[1] TREVOR HASTIE,[2] IAIN JOHNSTONE[3] AND ROBERT TIBSHIRANI[4]

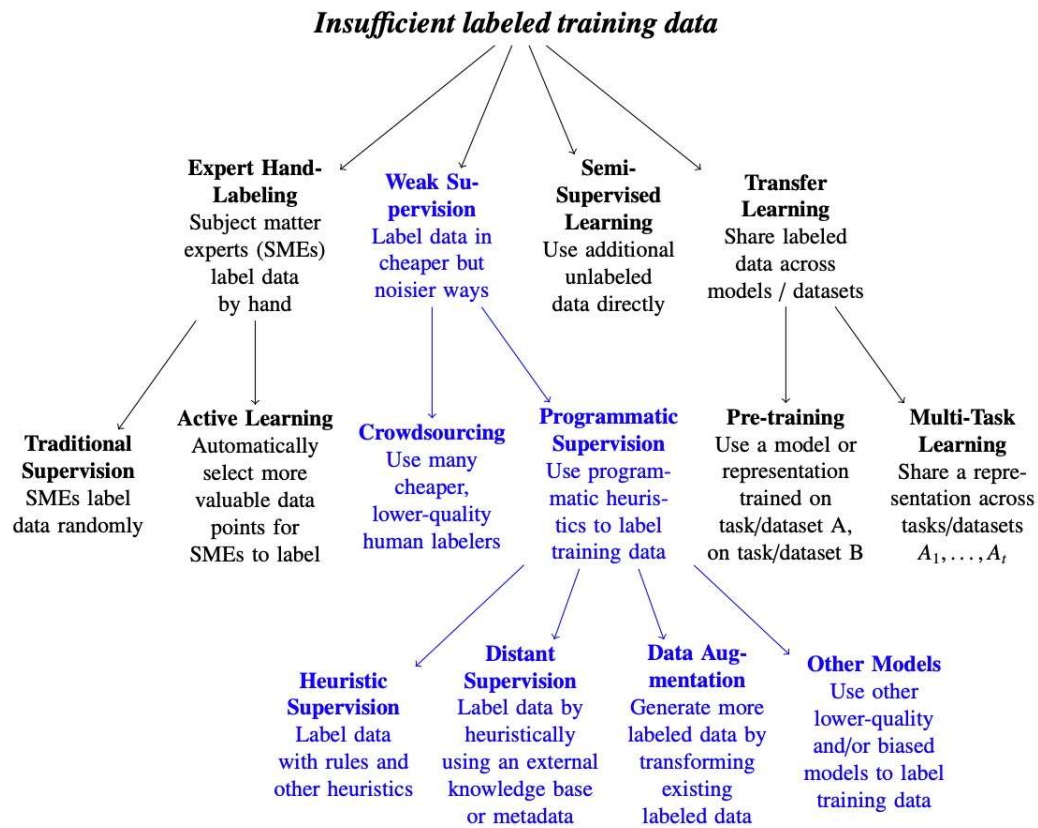
*Stanford University*




Useful to see how valuable each feature is: Great tool!

# Various techniques for limited labeled data

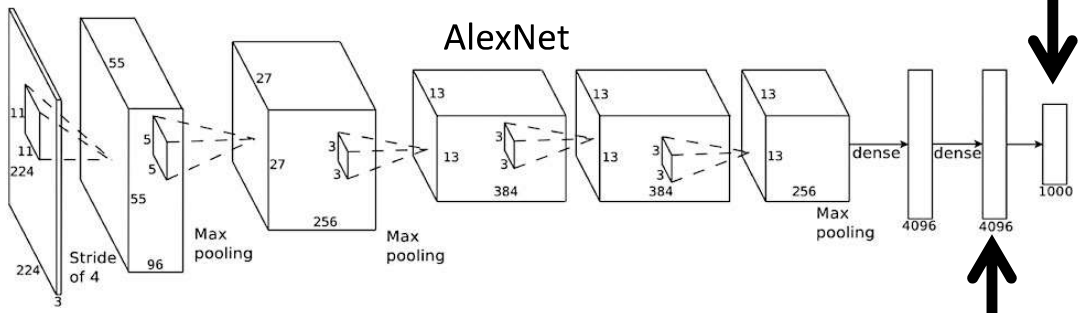
- **Active learning:** Select points to label more intelligently
- **Semi-supervised learning:** Use unlabeled data as well
- **Transfer learning:** Transfer from one training dataset to a new task
- **Weak supervision:** Label data in cheaper, higher-level ways




https://www.snorkel.org/blog/weak-supervision

# Transfer learning: Basic Idea

1000 classes in ImageNet, each component likelihood of class




Cat has highest value. (index 763)

A vector "representing" the image, features for "logistic regression".

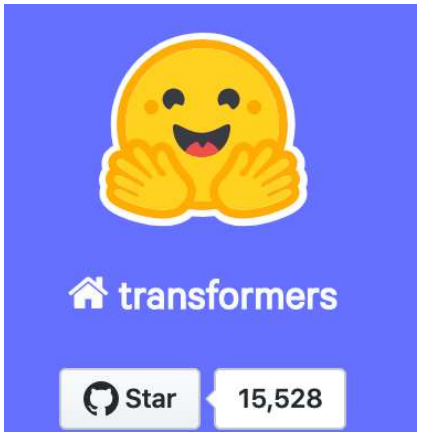
**Challenge**: Want to classify data into new classes—don't have 1M (picture, label) pairs. *Not enough data!*

**Transfer learning Idea**: *Can we just replace the last layer with our classes, and just retrain that part?*

***Abstractly**: A model can be viewed as a function from image to a vector.*

# Transfer learning for language

- Train (huge) models offline for language.
  - ELMO – UW, Allen
  - BERT -- Google
  - GPT-2 -- OpenAI
  - Roberta – Facebook
  - XLNet – Google/CMU



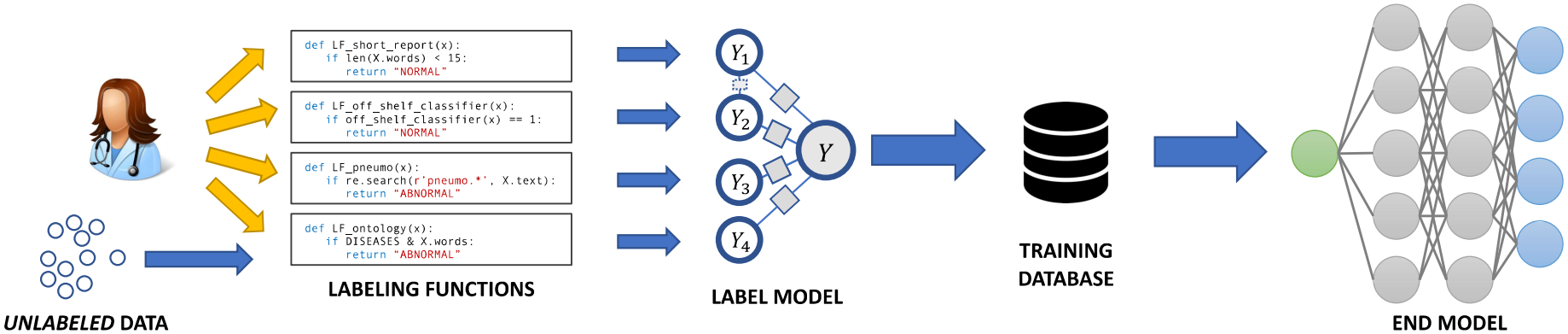

https://huggingface.co/transformers/

- Use trained representation (same last layer)—and simple refinement.
  - A great library with tutorials.
  - Outstanding way to get started with little data.

- **Key question**: If you have enough data for your task, pretraining shouldn't help.
  - Where is the cross over point? What is the performance cost?

# Weak Supervision Ex: Snorkel

snorkel.org



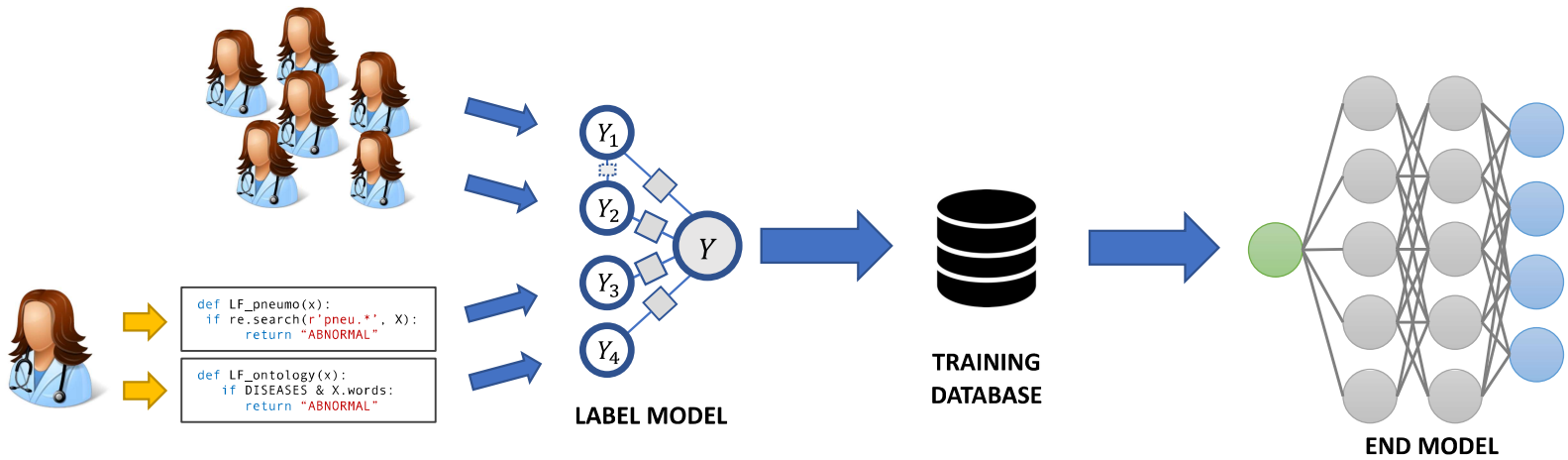

**Users write *labeling functions* to heuristically label data**

**Snorkel *cleans and combines* the LF labels**

**The resulting training database used to train an ML model**

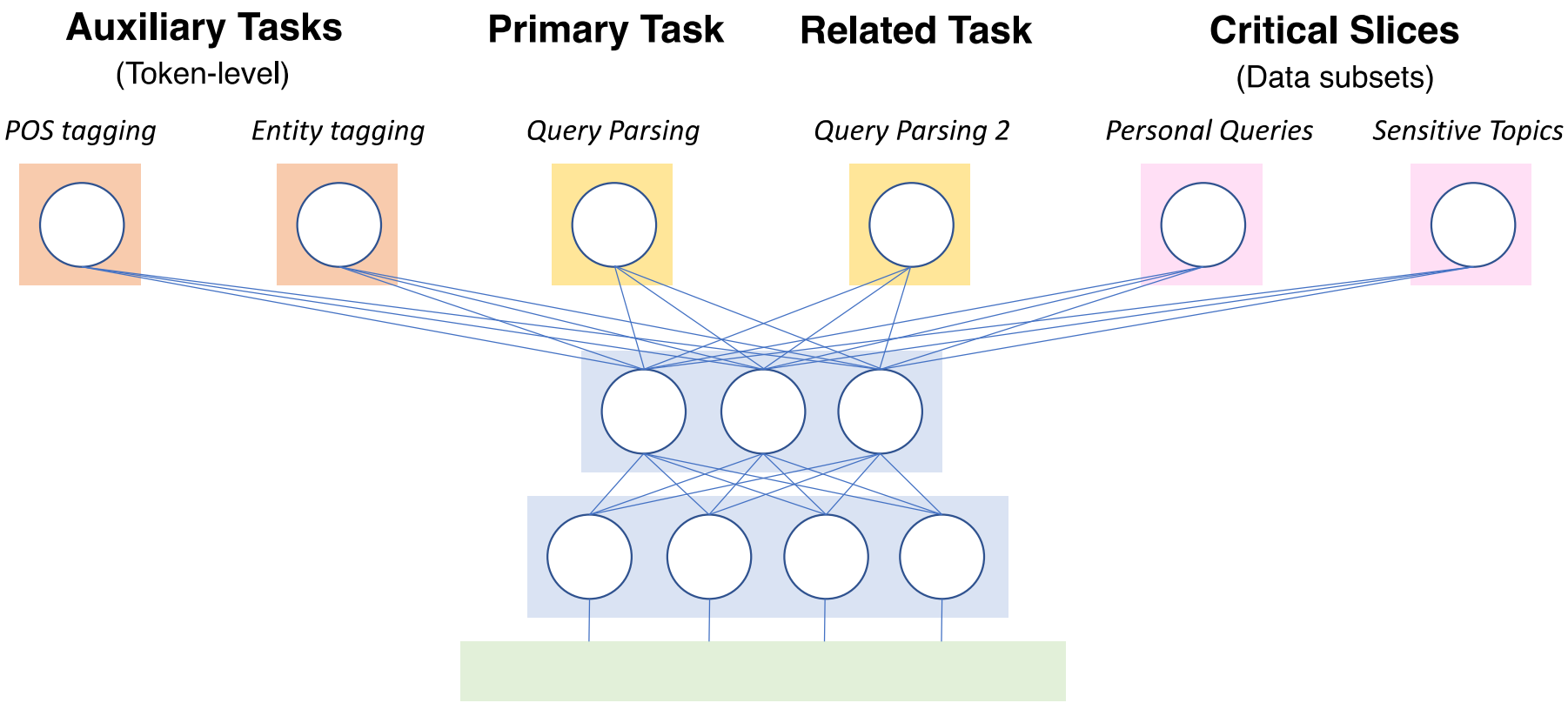
**Note: No hand-labeled training data!**

# Can subsume noisy “crowd” labeling as well




**“Hybrid” approaches use programmatic + human supervision**

# Massive Multi-Task Learning (MMTL)




**Capitalizing on supervision at every level of granularity**

# What changes with Foundation Models?

# Foundation Models and their change?

- Early, we still don't know.
- Foundations are meant to be *built* on.

- ChatGPT and other foundations.
  - First-mile v. last mile – I'm very much excited about this

- Big shift: Move from build-then-validate systems to validate-then-build.
  - h/t Chris Aberger, Numbers Station CEO

# Self-supervised Systems at Apple

In late 2017, enhancing a service that was doing NED (and QA,IE, topic rec)

- Completed high quality solutions for US English…
- Mostly deep model but had hand-tuned KG features, maintenance was an issue…

Apple overlords: Great! roll out to tens of locales…

*… but not tens of new head count…*

# Weaker forms of self-supervision

Remove manual bottlenecks with weaker forms of supervision.

- ELMO paper just came out (Feb 18). **Very inspiring!**
- Snorkel was getting traction at Google Ads.
- 1st version stomped our hand-tuned model (Early 18)
- But … integrated into Overton [CIDR20]…

1st cut model in production in 2018 (stayed there)
great quality bumps across locales, changed slightly over time, relearned weekly…*Woo hoo!*

# Foundation Models without Soylent (or AGI)

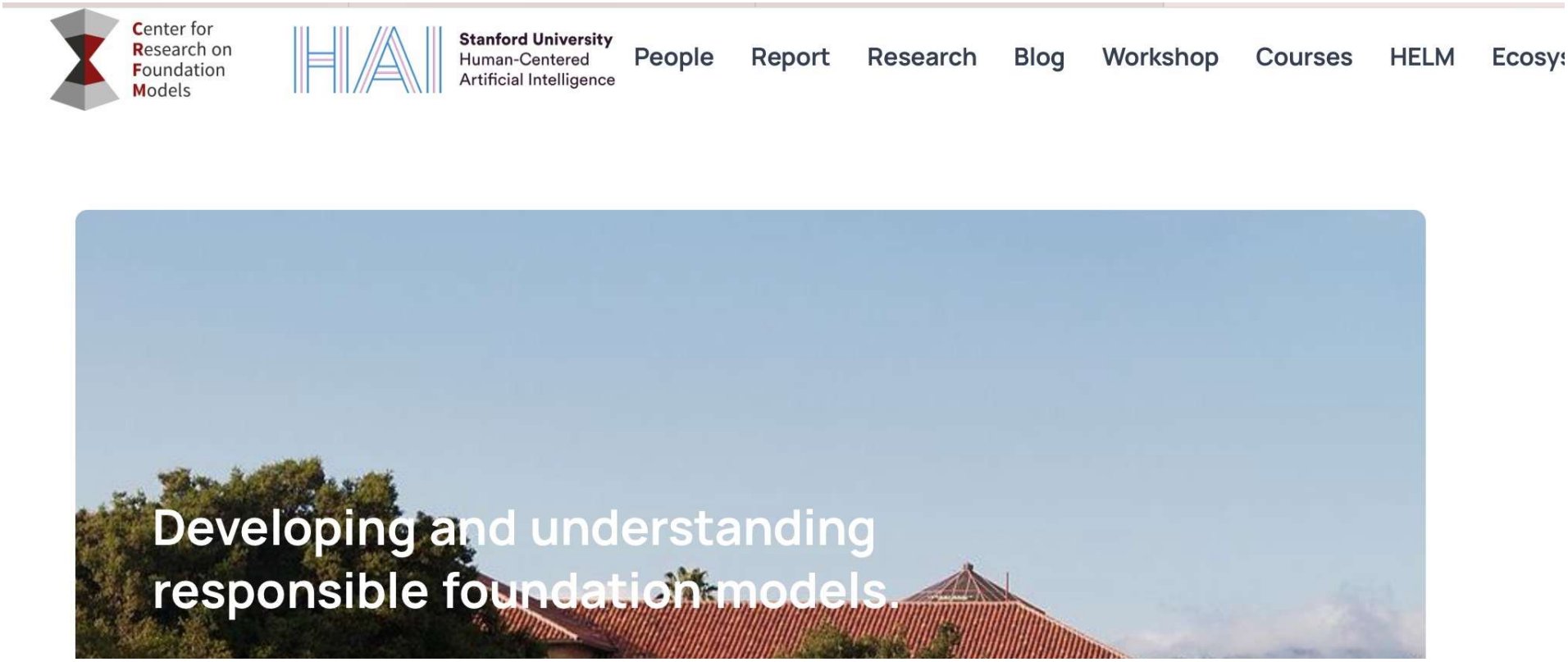
Practical reasons to love foundation models

**Sealed Engines:** Lots of small details in ML pipelines. Learned representations reduce engineers making irrelevant variations that break production.

- Ex: System I built trains itself each week for **years** (tens of FTE to 0.5 FTE to monitor).

**Death-By-A-Thousand-Cuts Problems:** In some problems, no *instance is hard per se*, but sheer variety of reasoning is.

- E.g., entity matching, always simple clues—but selecting right simple background knowledge is hard. (more later)



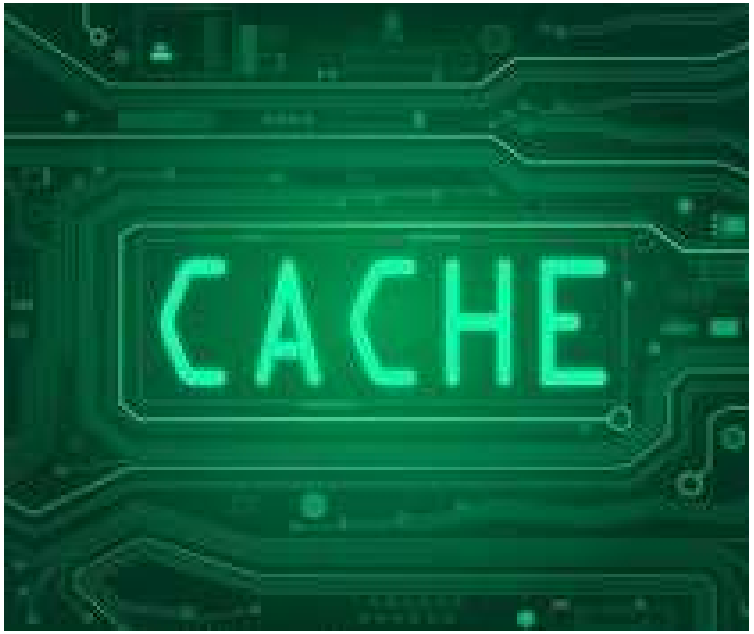

# This changed my view on AI + Systems

- Let me put toward founding CRFM
  - Center for Research on Foundation Models
  - https://crfm.stanford.edu.

# Production Issues

# Last line of defense: Caches and Overrides!

- Keep in mind, ML helps you build software. It's usually not a goal in and of itself.
- ML is not infallible.
  - If you can write it easily, just do it!
  - If it makes a mistake, put it in a cache!
- Danger: you incur technical debt or you avoid fixing actual issues in your model.
- Use sparingly, but used in most production systems.
- Hot fixes!



# Hidden Tech

## Hidden Technical Debt in Machine Learning Systems

**D. Sculley, Gary Holt, Daniel Golovin, Eugene Davydov, Todd Phillips**
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Google, Inc.

**Dietmar Ebner, Vinay Chaudhary, Michael Young, Jean-François Crespo, Dan Dennison**
{ebner,vchaudhary,mwyoung,jfcrespo,dennison}@google.com
Google, Inc.

# Hidden technical debt.

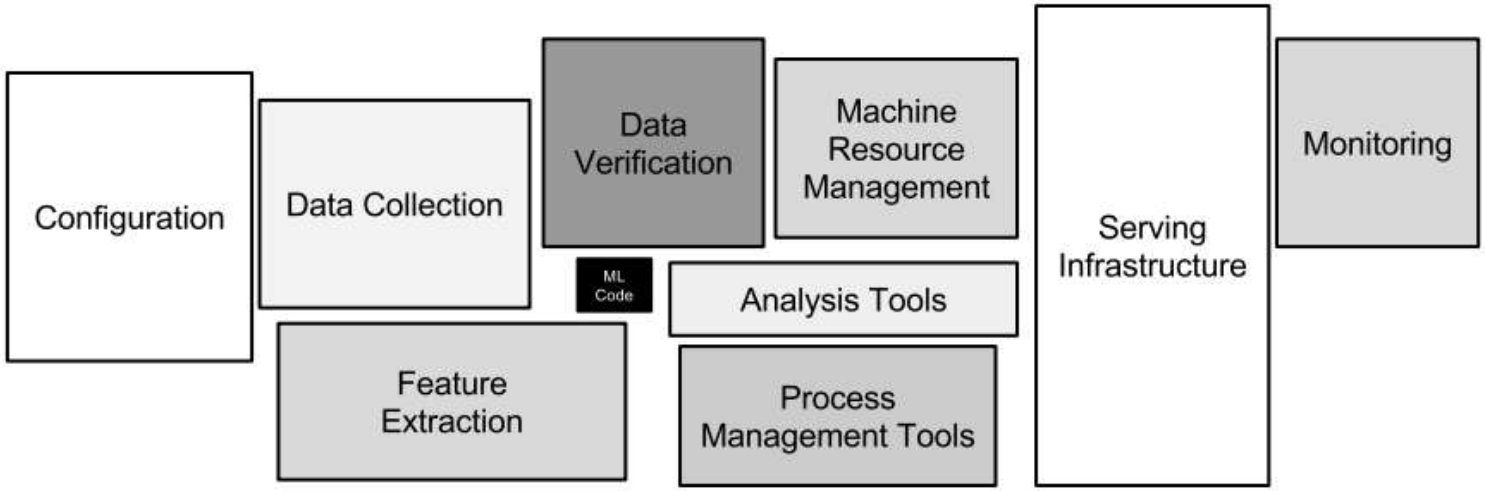



Figure 1: Only a small fraction of real-world ML systems is composed of the ML code, as shown by the small black box in the middle. The required surrounding infrastructure is vast and complex.

# Code is nasty

- In conventional code,  the person who wrote it usually knows why it works—but maybe no one else!

- In ML code, no one may know!

# Hidden Benefit of Neural Nets

- Representation and normalization code is nasty. I've yet to see someone proud of it.
  - In a NN, you relearn it, and so don't have to maintain it.

- ML is eating software!

- This is called Software 2.0
  - Andrej Karpathy
  - Disclosure: We also work on this a lot!

https://arxiv.org/abs/1909.05372

# Overton: A Data System for Monitoring and Improving Machine-Learned Products

Christopher Ré
Apple

Feng Niu
Apple

Pallavi Gudipati
Apple

Charles Srisuwananukorn
Apple

Raising abstraction and focus on monitoring rather than building models.

# Reproducibility

***Reproducible, Reusable, and Robust Reinforcement Learning***

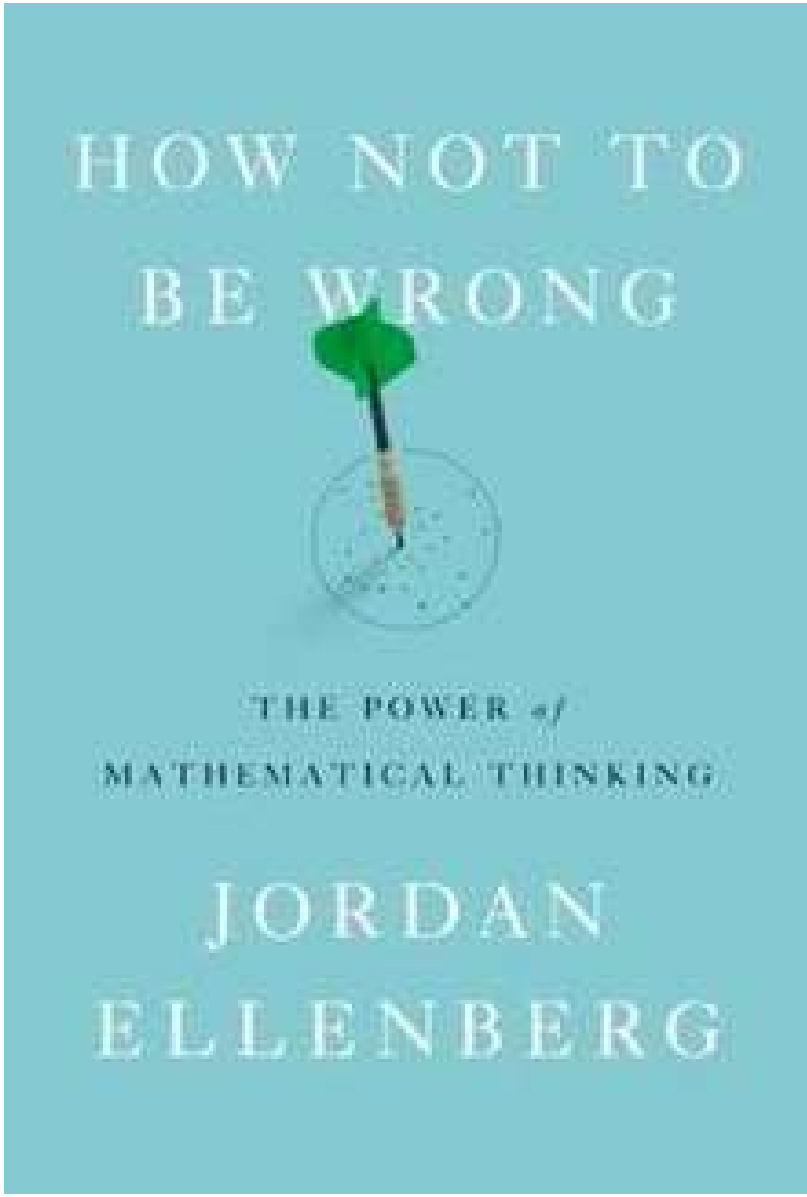
**Joelle Pineau**
Facebook AI Research, Montreal
School of Computer Science, McGill University

Neural Information Processing Systems (NeurIPS)
December 5, 2018

Great talk! Highly recommend it
(Keynote last year—Kunle was great too!)

# Reproducibility

- Your goal is to avoid fooling yourself.
  - It will be hard! You're clever!
- **Meaningless change causes a quality change:** Random seeds shouldn't matter, but they lead to different outcomes!
- We separate train and test in an effort to not be wrong.
- No silver bullet, diligence everywhere.



# Anti-Reproducibility (Crisis) in FMs?

- I don't have much to say, but one area of technology that is amazing is for **foundation models**—these things seem to be reproducible!
  - Many groups getting close to same results. It's amazing!
  - It's really exciting to see!

- People worried they are too easy to deploy and train! Leading to open source AI for FMs?
  - Blog about AI's Linux Moment

# Summary

# Summary

- Measure twice, cut once. Don’t bash, try to setup diagnostics.
  - Ideally in code! You want to reuse these!
- Look at your data and your predictions. No substitute.
- ML systems are used to make it easier to write code, it’s a *“high-interest credit card of technical debt.”*