

ML Advice (Clipart day)

Chris Ré
with help from Alex Ratner

Disclaimer

- This lecture is filled **with personal opinion** informed by building production and clinical prototypes (and research too!).
- It is high level and presents some difficult, raw material.
- **Improve over time:** include ideas folks have told me were helpful to them.

Disclaimer

A magnifying glass with a black handle and a silver frame is positioned over the word "Disclaimer". The lens is focused on the letter "D", while the rest of the word is visible through the glass.

- 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 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...



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.



Upshot:
Picked up on
mascara

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

Hidden data artifacts are very challenging!

Step 2: Look at the data

Look at your data.

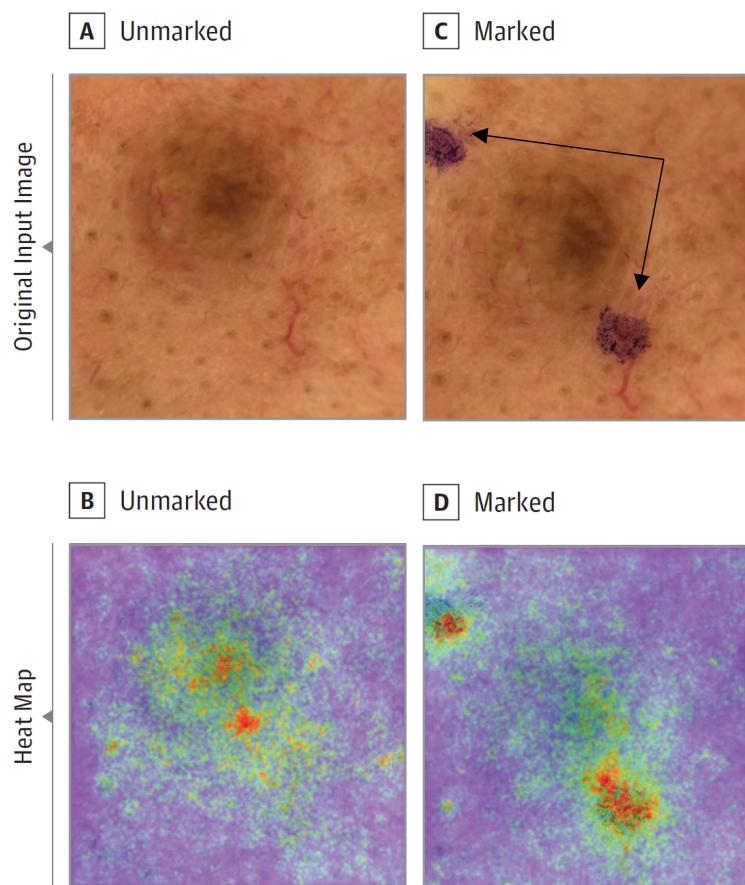
- You have some spam, look it at it!
- If needed, build tools to look at your data.
 - Spam from Europe different than from Africa? from US?
 - Spam to .edu different than .com?
- “Become one with the data” – Karpathy.
- Do this at every stage!



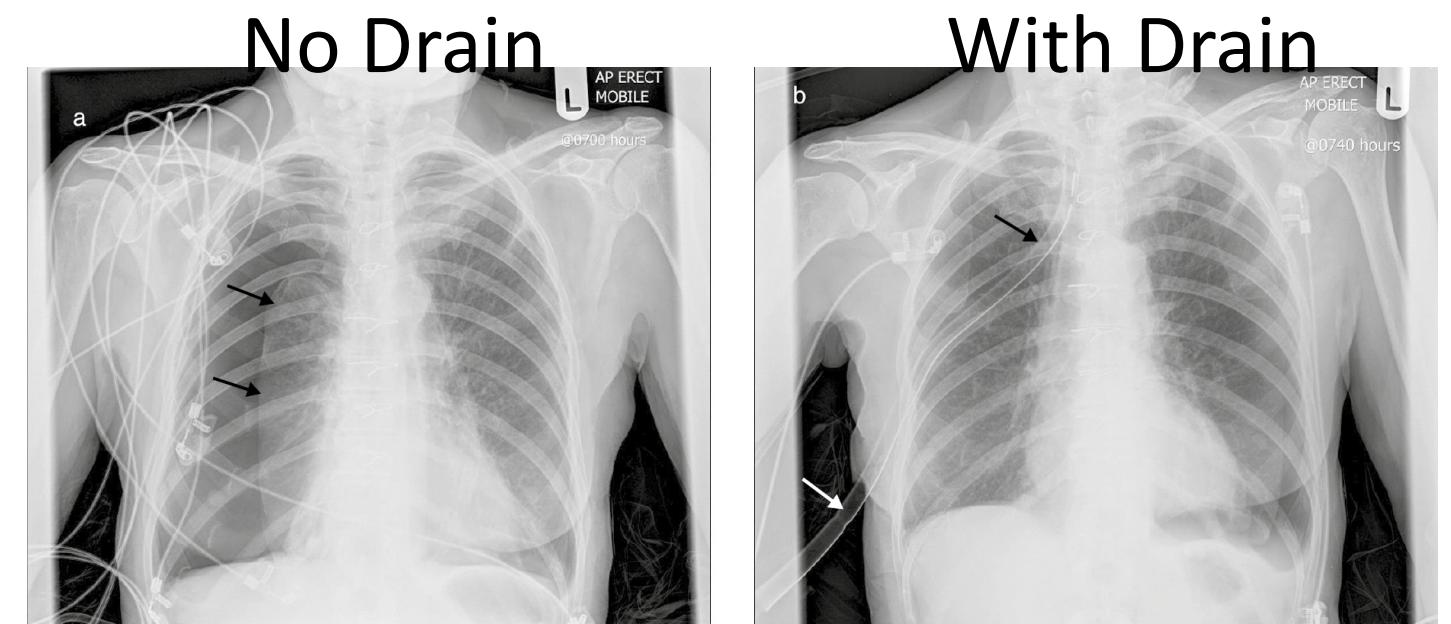
Have the right people look at your data

Expertise is often required!

Melanoma Recognition (Surgical Marks)



Pneumonia Detection (Chest Drains)



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

Image Credits

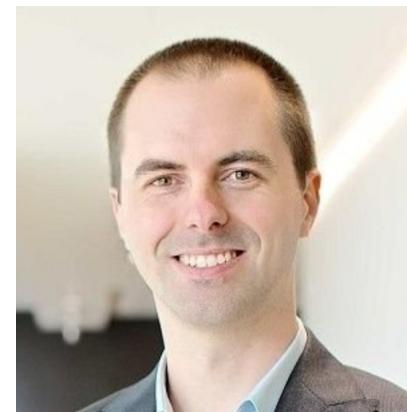
Valchanov, Kamen, Nicola Jones, and Charles W. Hogue, eds. *Core Topics in Cardiothoracic Critical Care*. Cambridge University Press, 2018.
Winkler, Julia K., et al. "Association between surgical skin markings in dermoscopic images and diagnostic performance of a deep learning convolutional neural network 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)

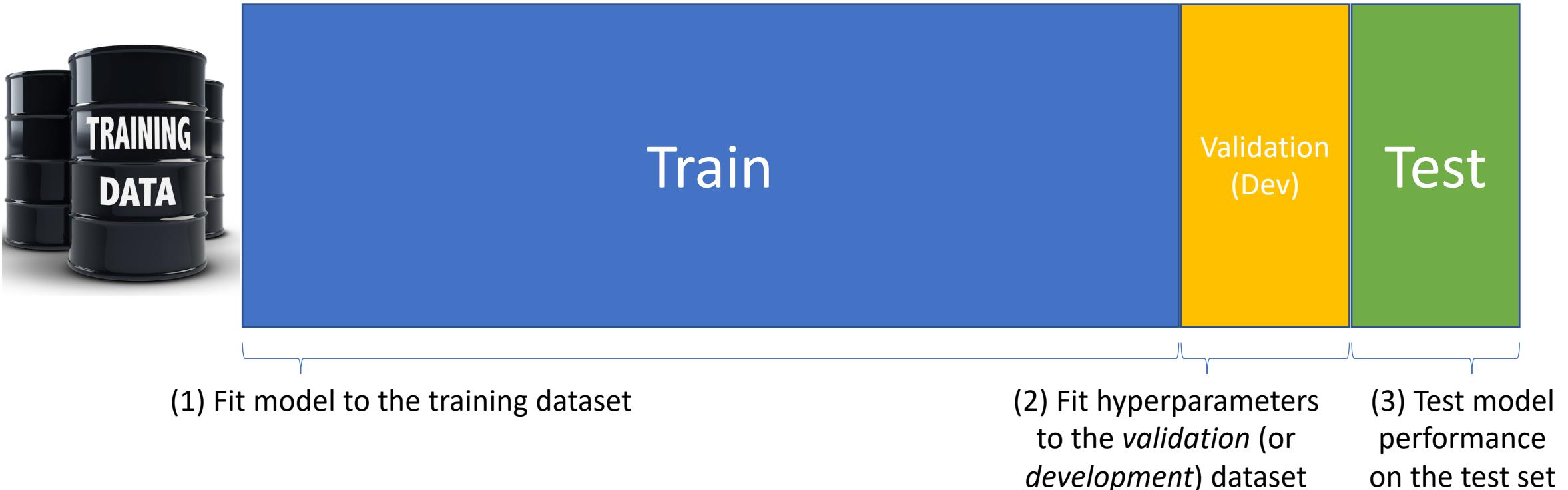


Jared Dunnmon (Stanford)

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

Step 3: Train/Dev/Test Split

Partitioning Data: Train, Test, and Validation



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
- 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?



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!**



A **test set** is an important part of your specification.

Quick and Dirty Test: Inner Annotator Agreement

- You write down your notion of SPAM. Select N randomly selected examples. Give to three different annotators.
 - **Inner annotator agreement.** How often do they agree?
- Let's say they agree 95% of the time—sounds 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...



Subtle
Problem:
*Consistency in
test sets*

Consider following protocol.

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

Subtle Problem: Spec creep



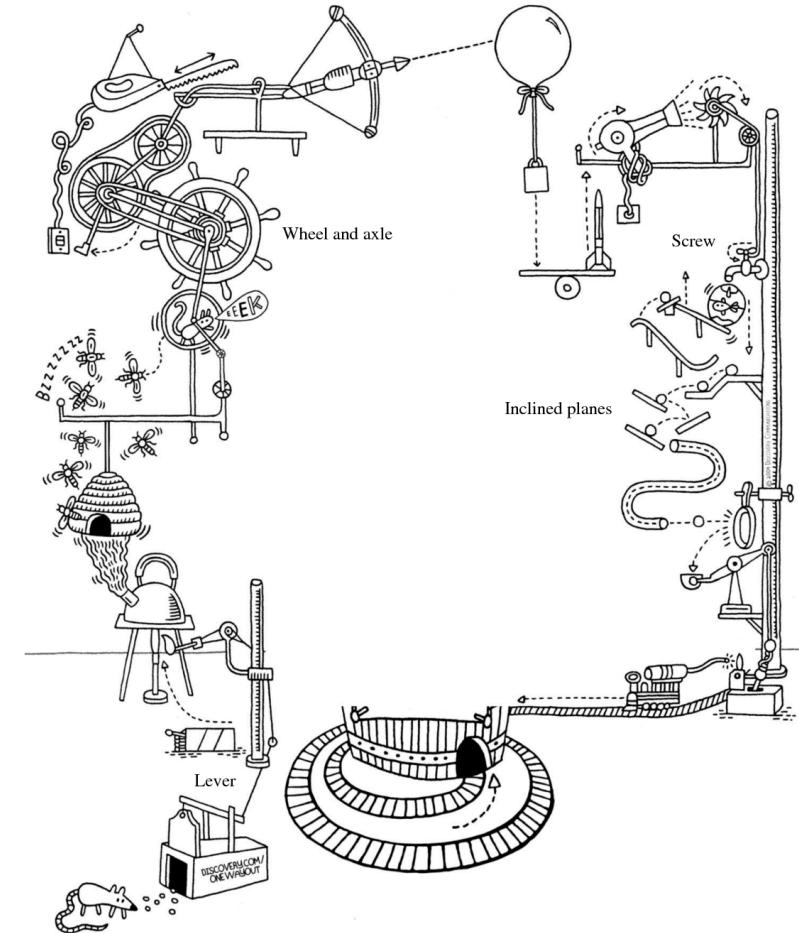
- **Warning:** Tempted when answer is “*pretty good*” to say yes—for classification this must be precise or you accrue debt.
- **Spec:** Unsolicited drug ads should be marked drug spam.
- Spam for vitamins comes in—and is successfully filtered.
- This answer is marked as drugs and filtered.
 - Answer is useful, but allowing it may cause **scope creep**.
 - If you want, it revise the specification.

Step 5: Implement simplest possible model

Keep it simple!

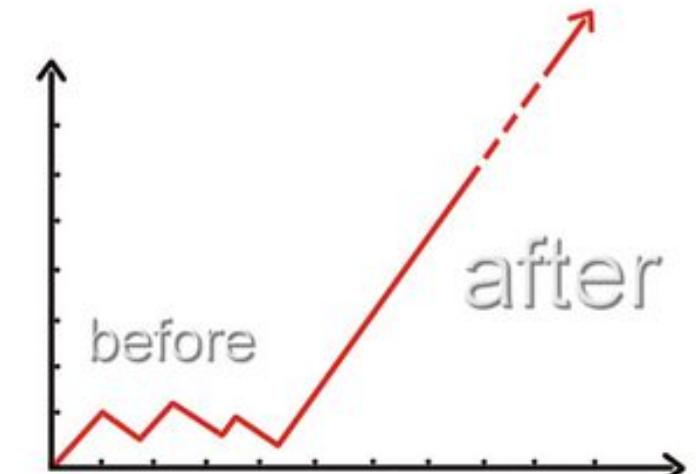
- If python code can get 90% accuracy, use it!
- If python code can get 100% accuracy, use it!
- ML shines on a class problems:
 - That can be **precisely specified** but
 - Writing down program is prohibitively hard
- **Avoid getting bogged down in models, use them to understand the data!**

Rube Goldberg Design Project



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...
- ***Build simpler methods even after fancy models.*** Often use deep models to “come up with features” – by looking at output!
 - Models are 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?



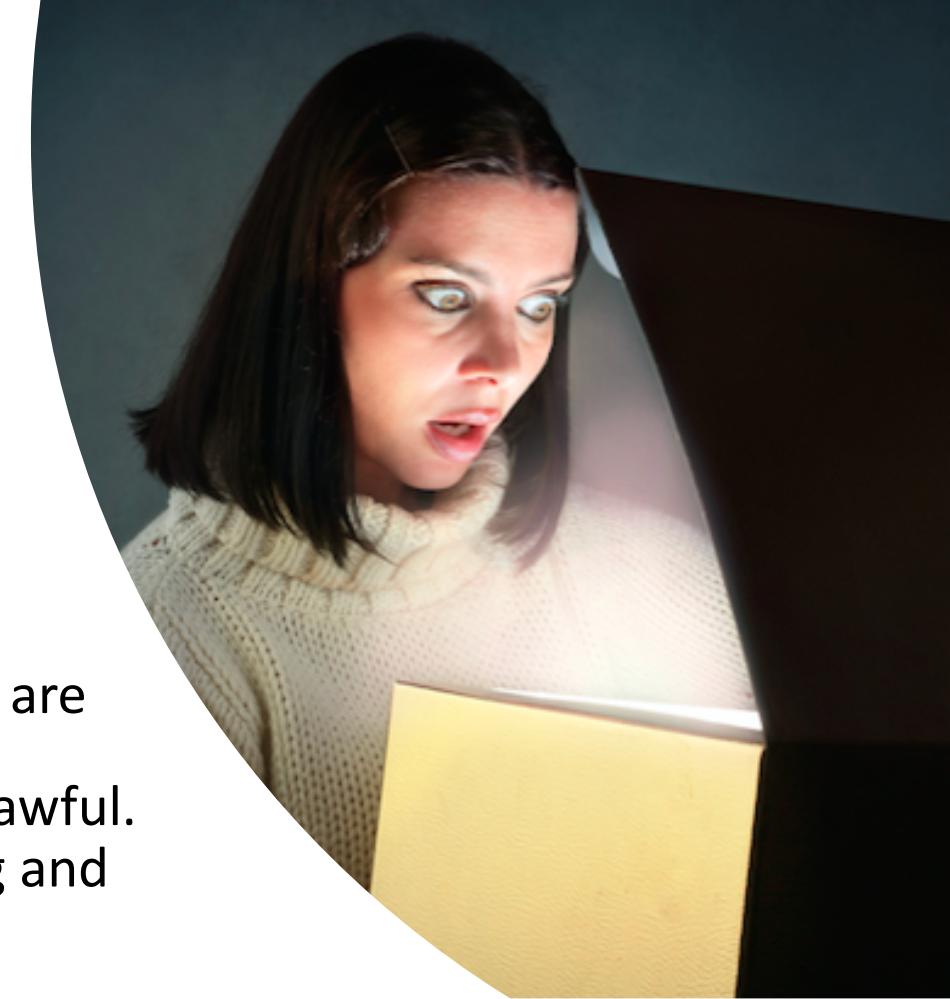
Avoid Known mistakes Slice-based Monitoring.

- 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!



Challenge: Avoid *unknown* mistakes

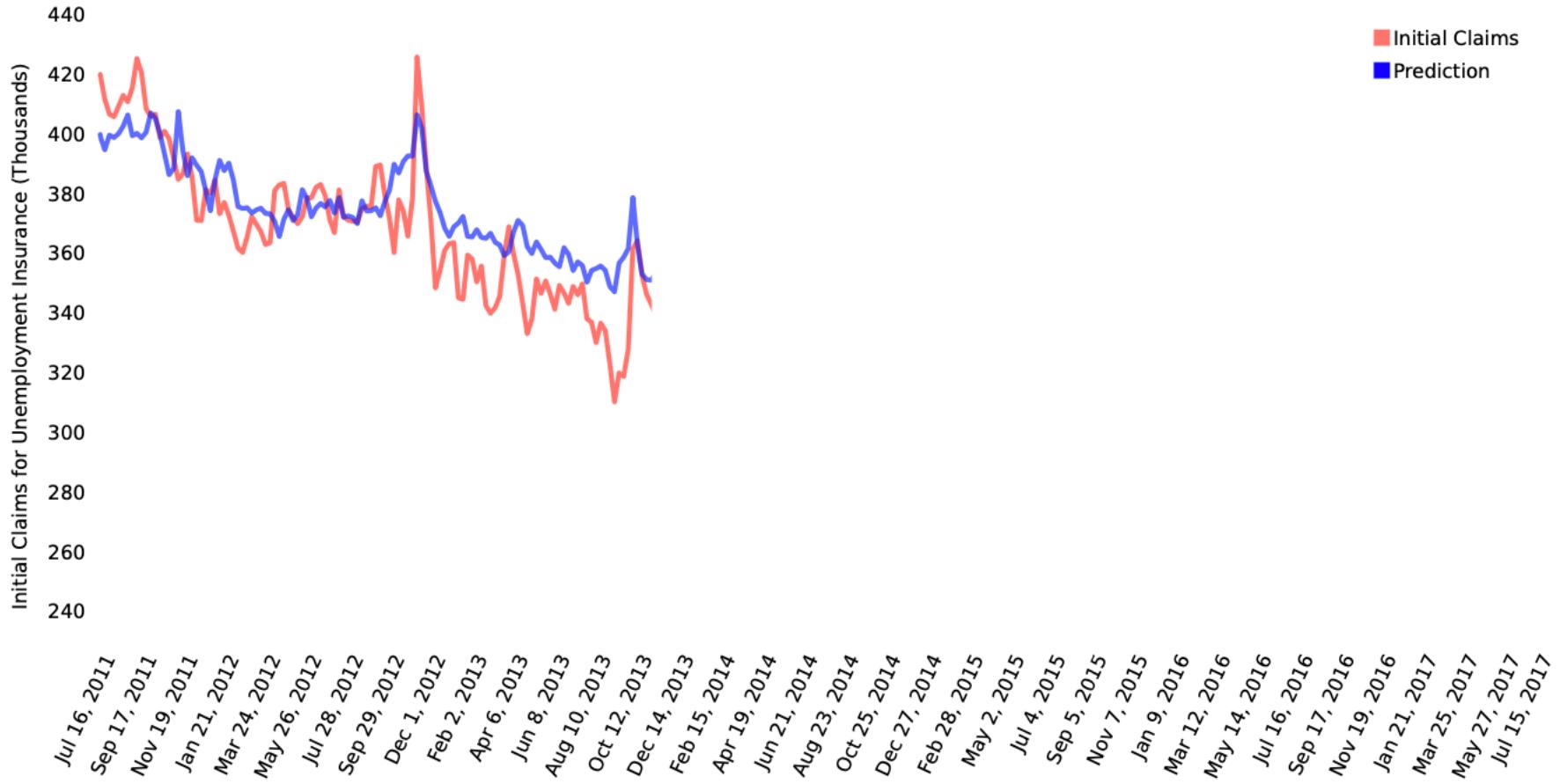
- Distribution shift is a real issue.
 - **Popularity Shift/Cold-start.**
 - You release a feature, queries that weren't popular are now **very popular**.
 - Old score says "we're great", but felt experience is awful.
 - **Remedy:** Hopefully, you knew this slice was coming and you monitored it proactively.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



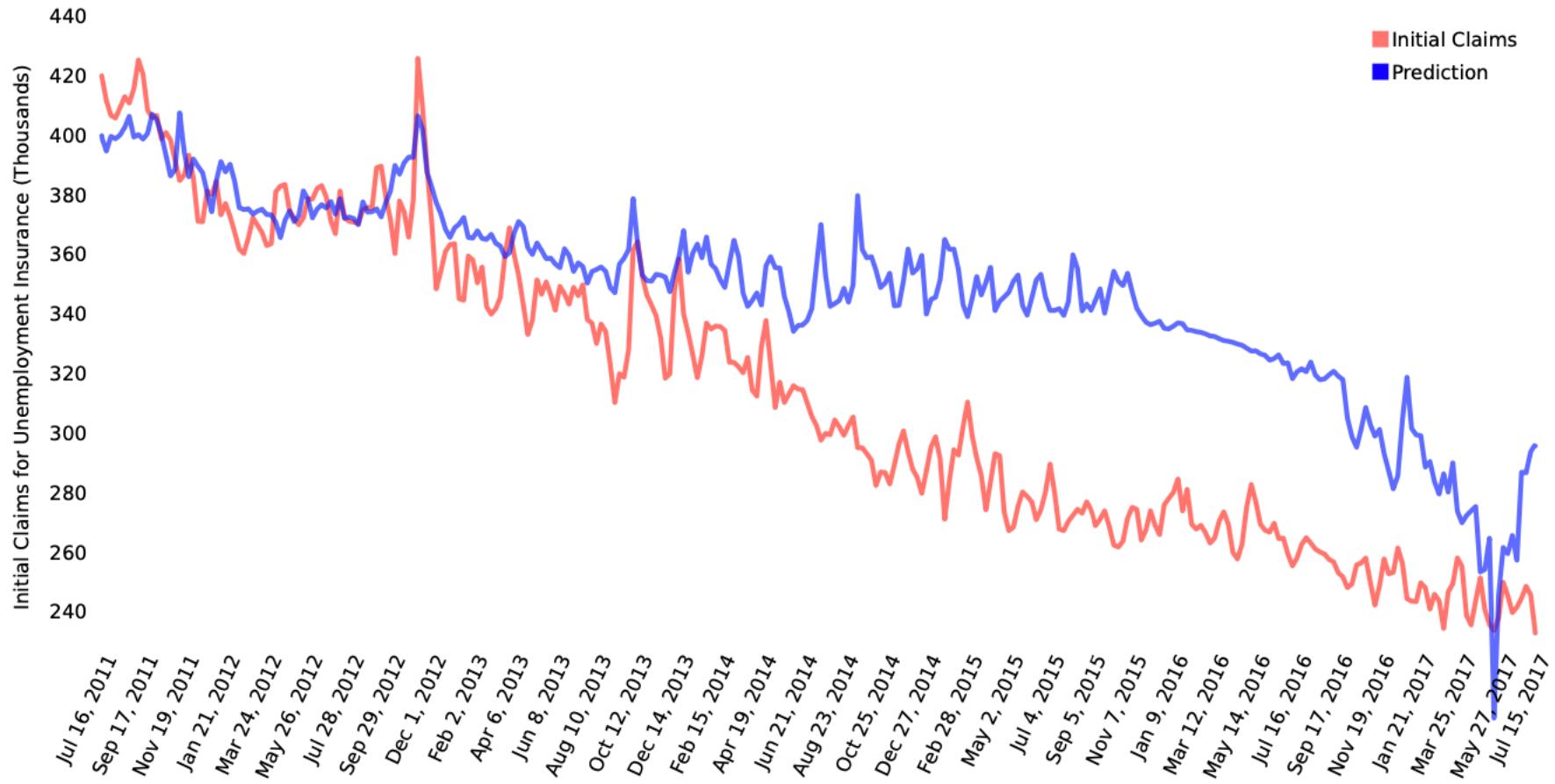
This is incredibly hard! No ideal solutions in industry...

*I've gotten this **very** wrong...*

Predicting unemployment claims from Twitter (at time of publication)



Predicting unemployment claims from Twitter (post-publication)



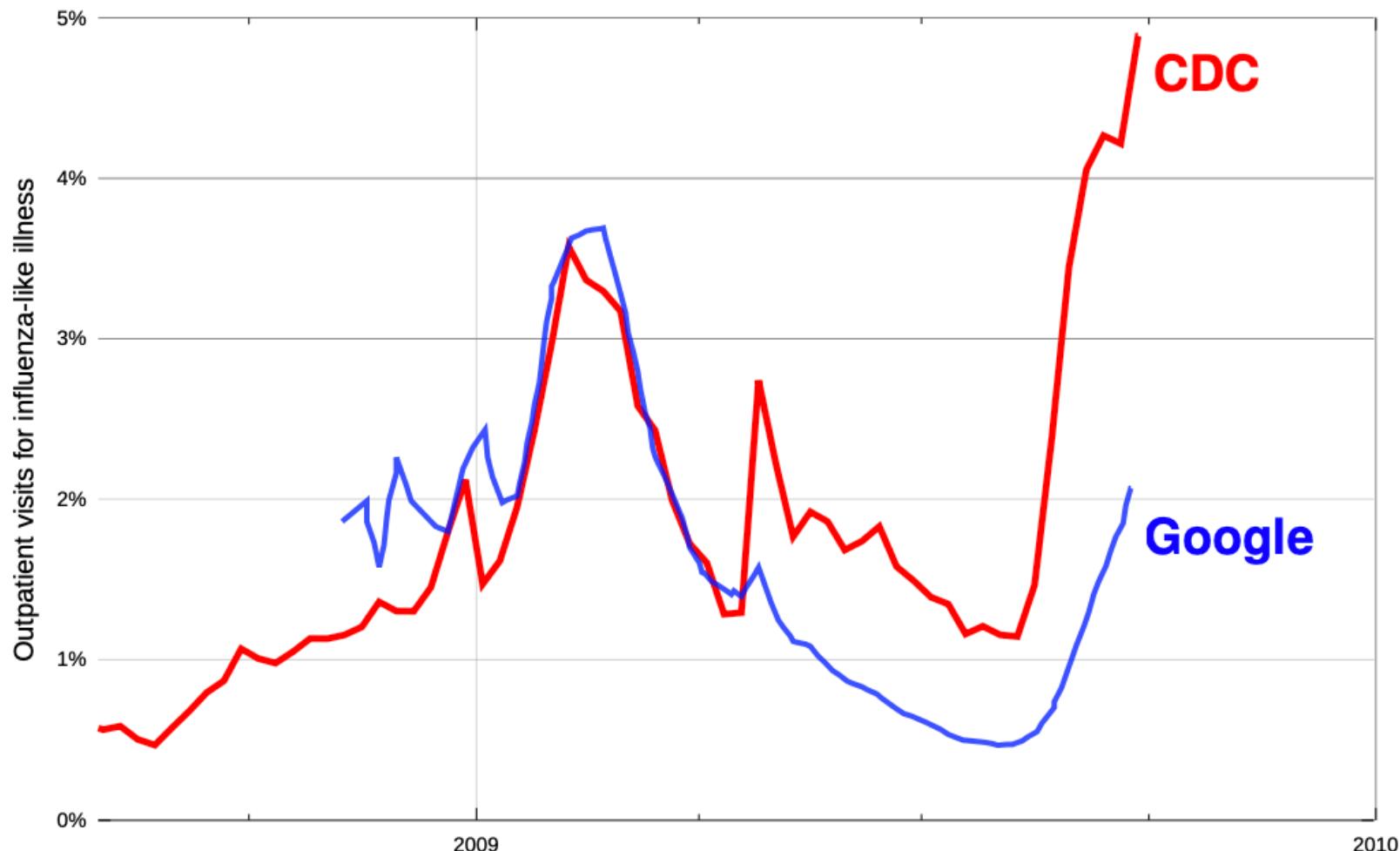
What went wrong?!?

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 a technique called PCA that we'll see in a few lectures to help...*

Performance in the first year





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
- Step 4: Create/Refine a specification
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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....

A screenshot of a Google Sheets interface. The title bar says "Example Sheets Add-on". The menu bar includes File, Edit, View, Insert, Format, Data, Tools, Add-ons, and Help. A sidebar titled "Example Sidebar" is open, containing the text: "This sidebar allows you to pull a value from a cell into the sidebar and place a value from the sidebar into a cell." Below this is a "Sidebar value:" input field with the value "1", and two buttons: "Pull" and "Put". The main spreadsheet area shows a single row with columns A, B, C, and D. Cell A1 contains the value "1". The bottom right corner of the spreadsheet has a link: "Sheets Add-on Template by Google".



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!

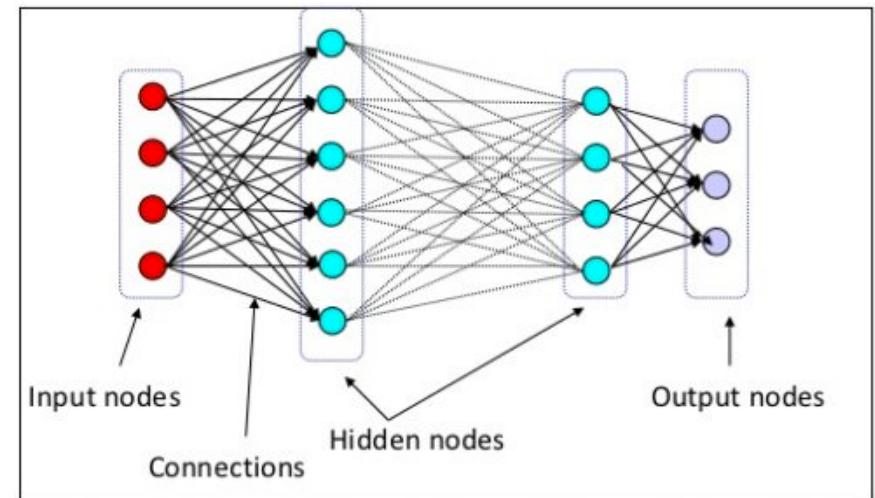
Selecting more labels

- It's all about sampling!
- Uniform Random Sampling
 - 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!
 - 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

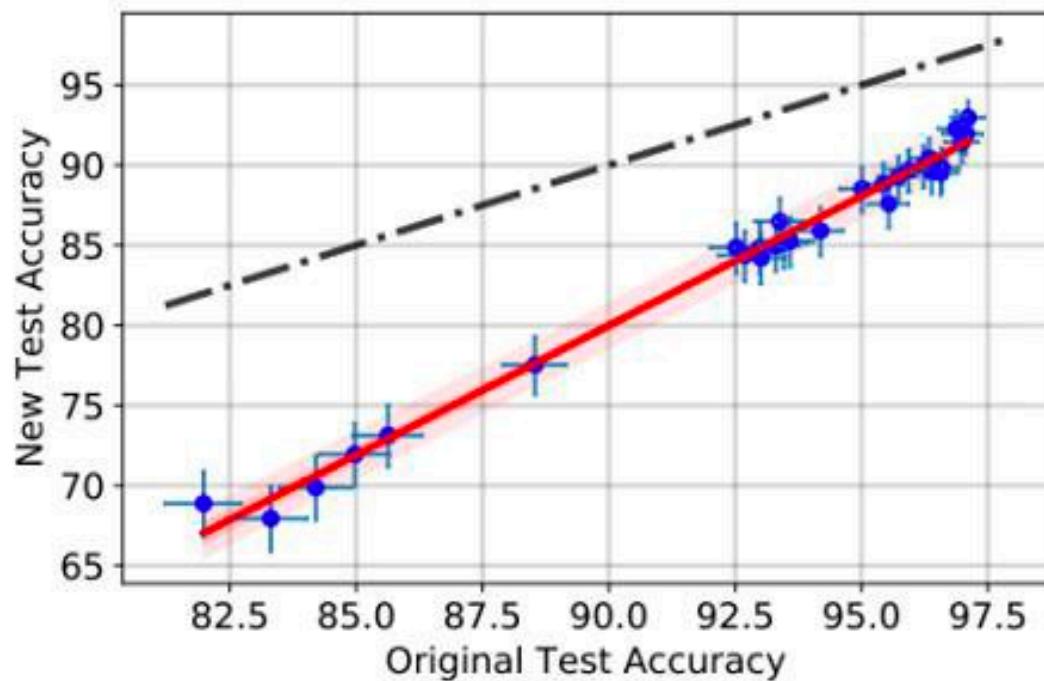
June 4, 2018

Do ImageNet Classifiers Generalize to ImageNet?

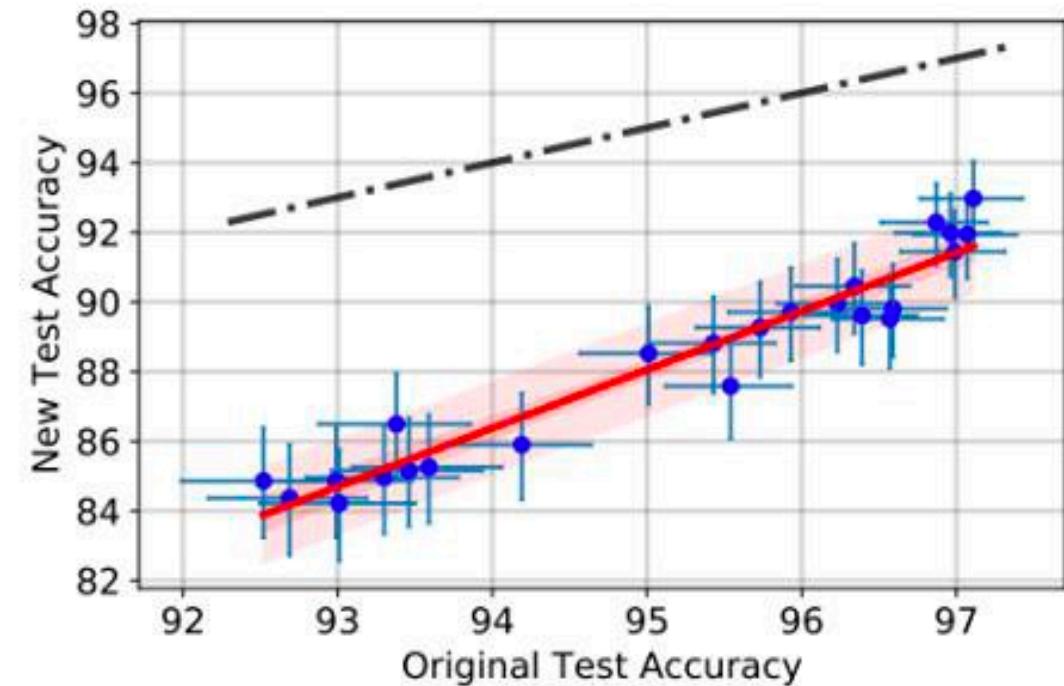
What if we sampled a new test set according
to the same specification as the original?

Expect the same outcome!

No real evidence of adaptive overfitting!



(a) All models

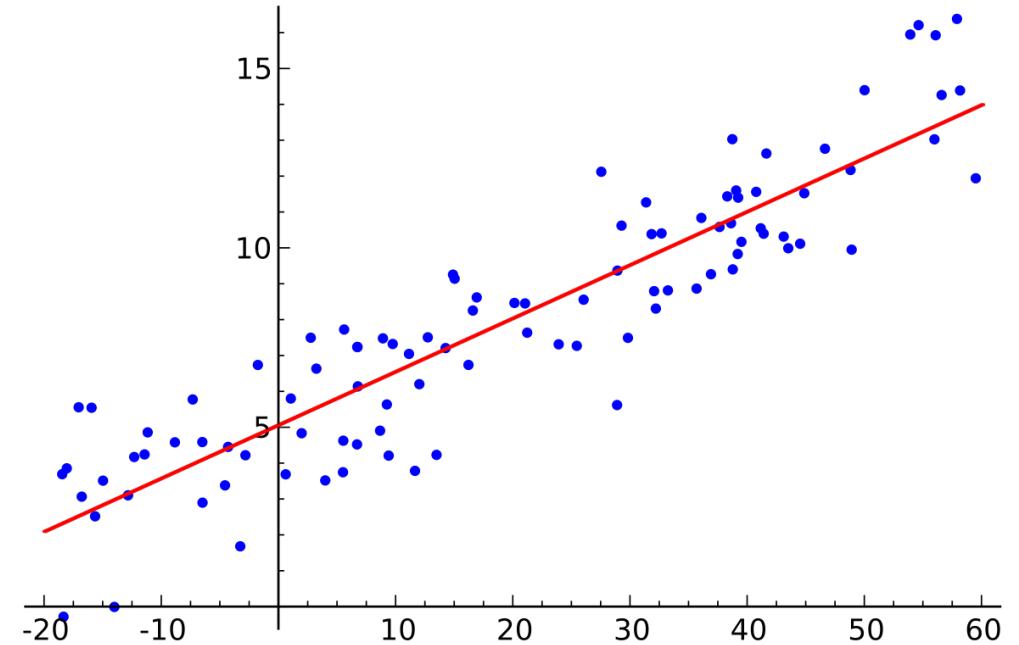
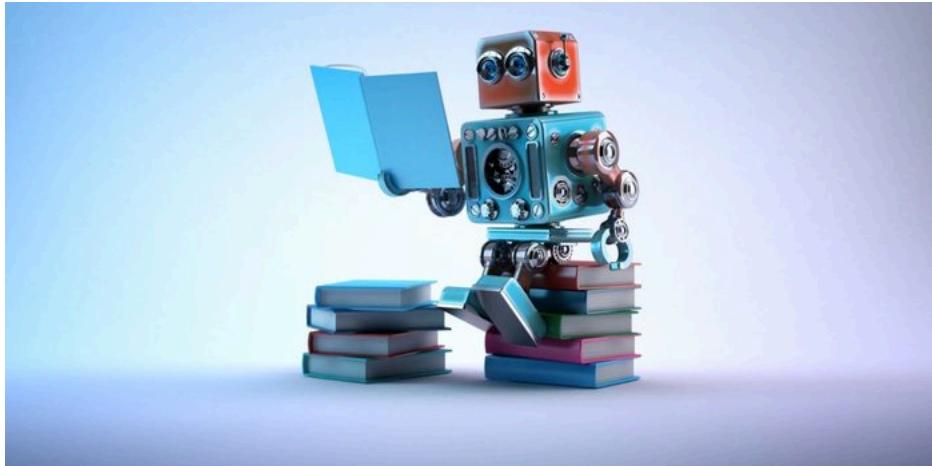


(b) High accuracy models

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 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, its error is too high!
- What do you do?



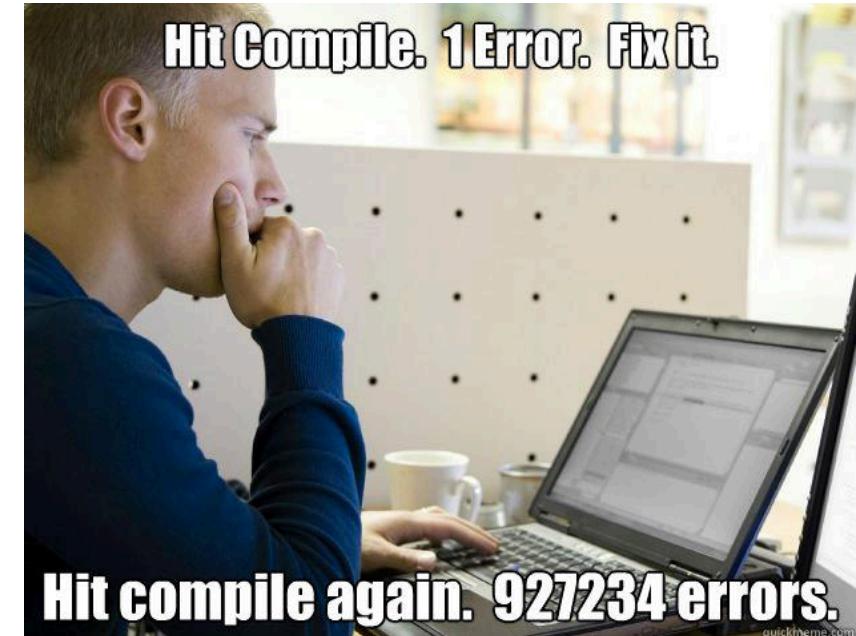
What could be wrong?

- 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?'**

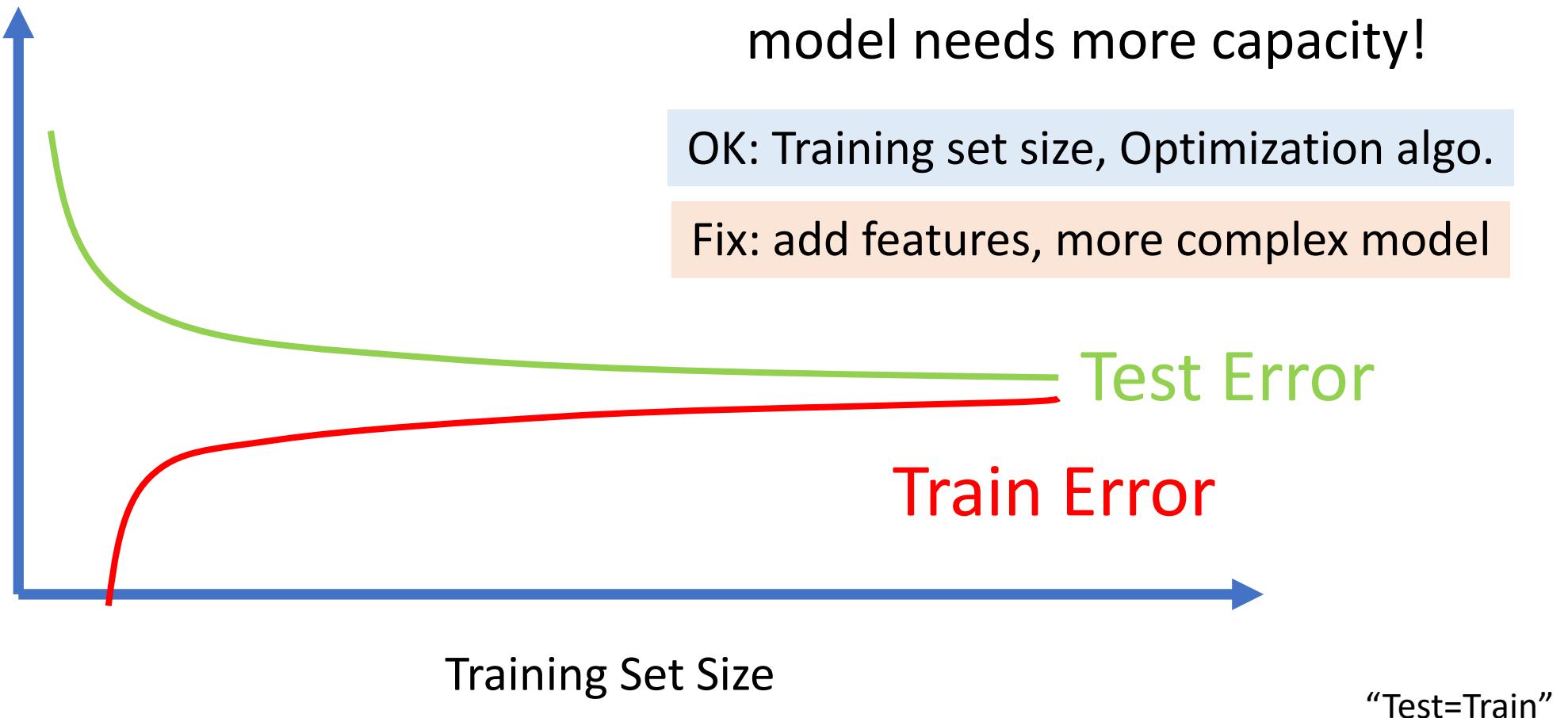
Just like compiling!

- 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!

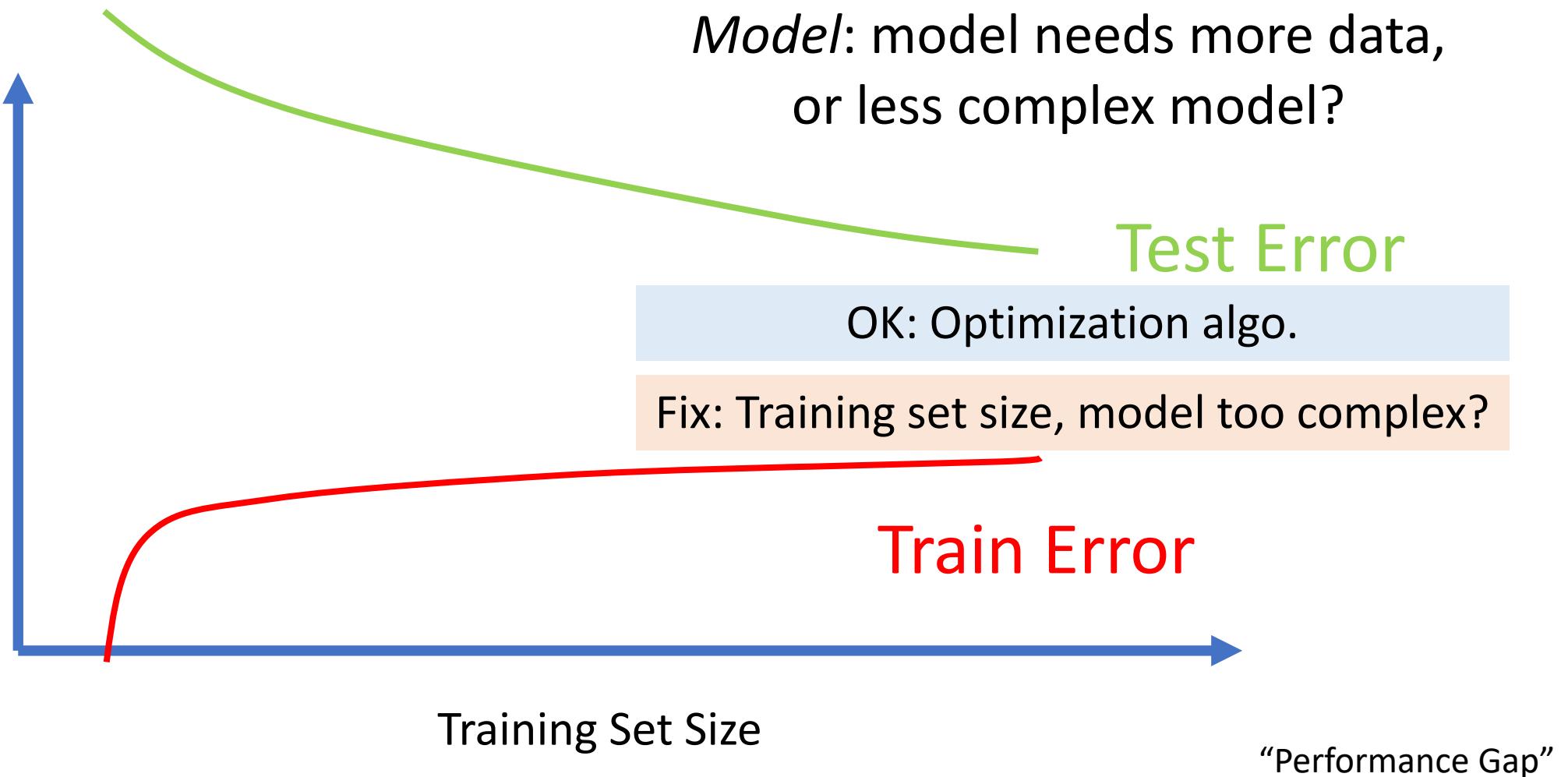


We'll cover some diagnostics that have helped us.

Diagnostic: Test versus Train Score.



Diagnostic: Test versus Train Score.



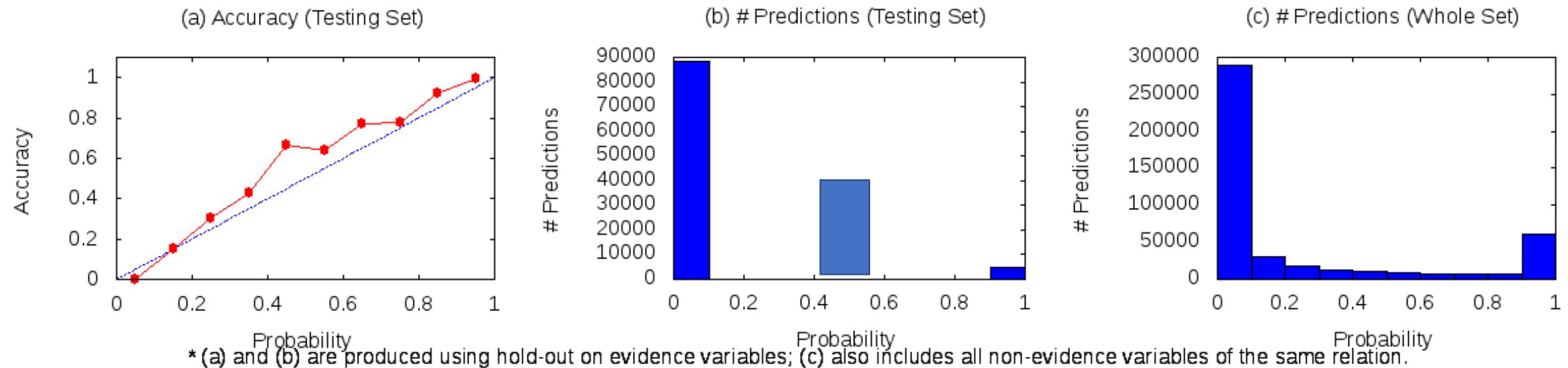
Variance Diagnostic

- 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 your target error is 10%, and your variance $\sim 1\%$ 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)



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 $\text{train} == \text{test}$
 - Fix: you need a more complex model.
- If $\text{train} < \text{test}$ 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.



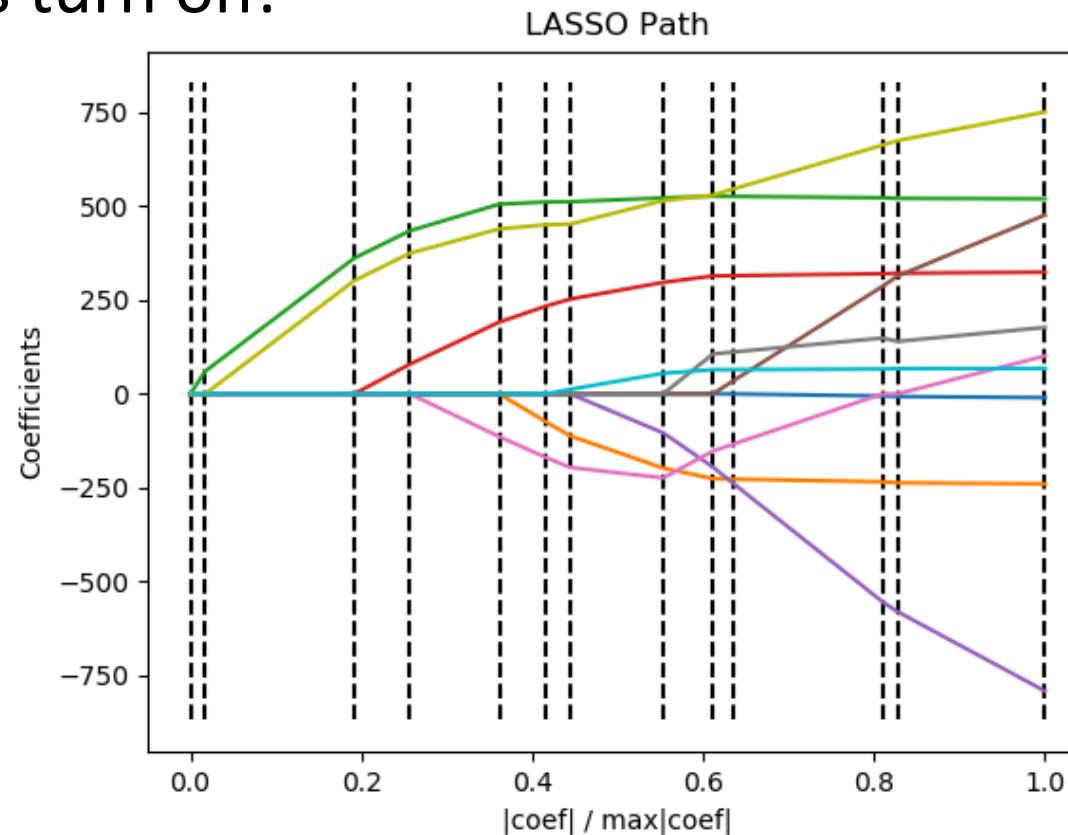
Lasso Path

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 JOHNSTONE³
AND ROBERT TIBSHIRANI⁴

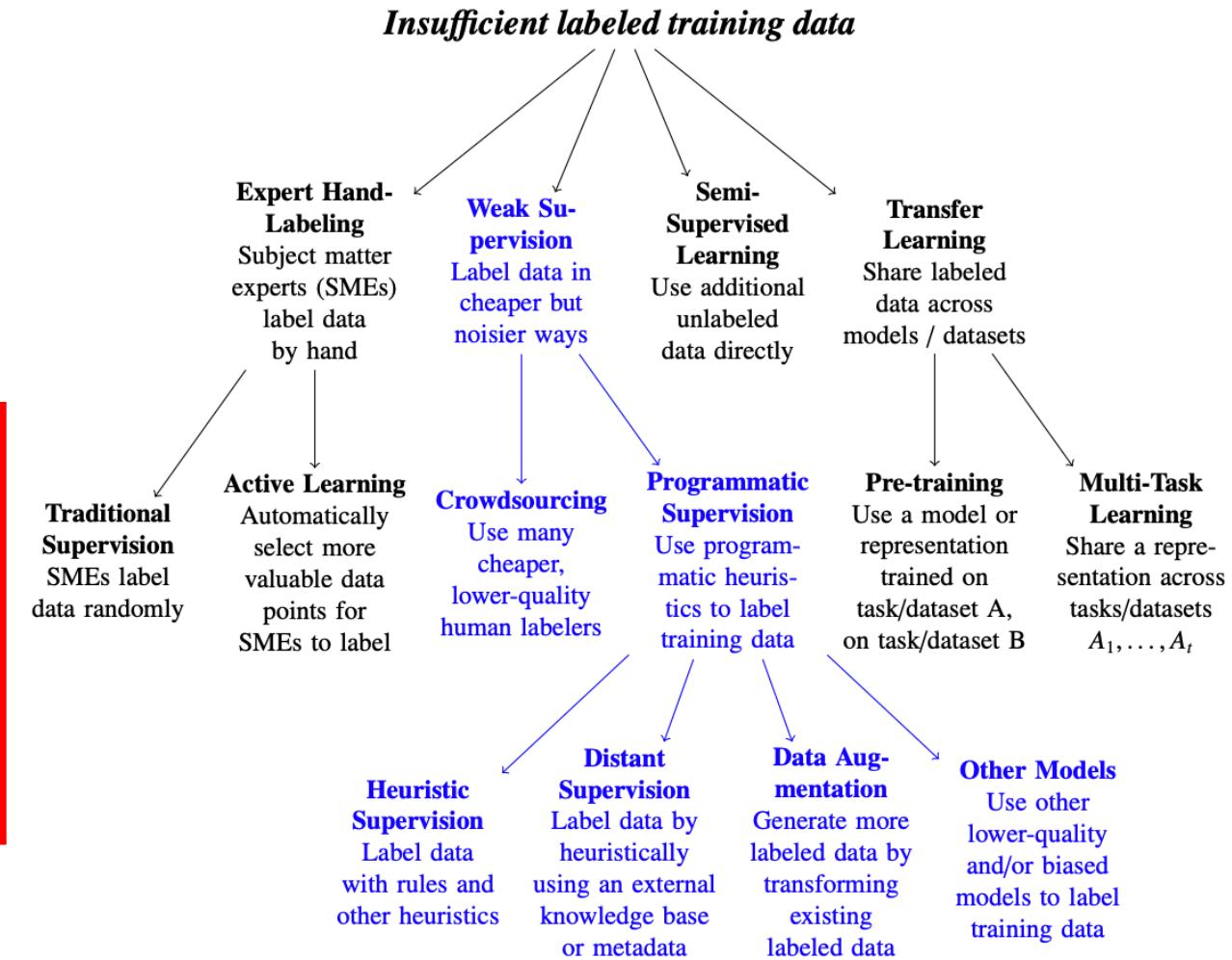
Stanford University



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

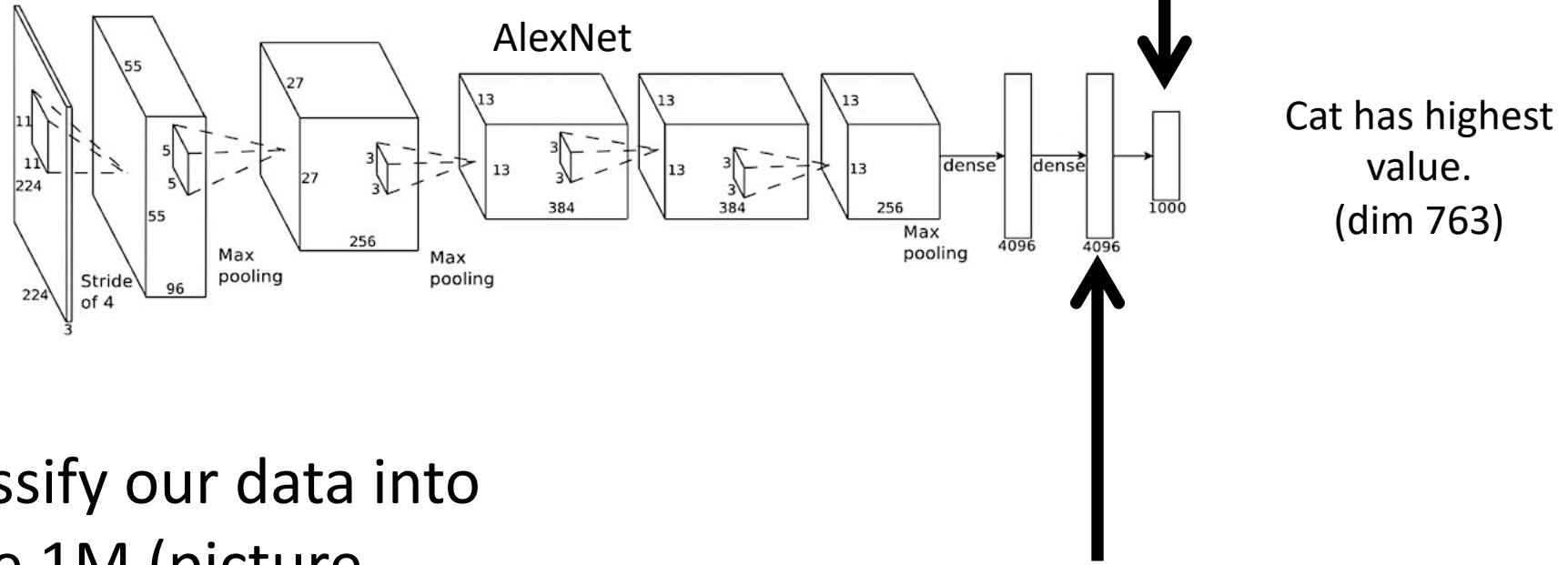
Various techniques for limited labeled data

- **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



More in lecture 20

Transfer learning: Basic Idea



Challenge: Want to classify our 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?*

1000 classes in ImageNet,
votes how likely in each class

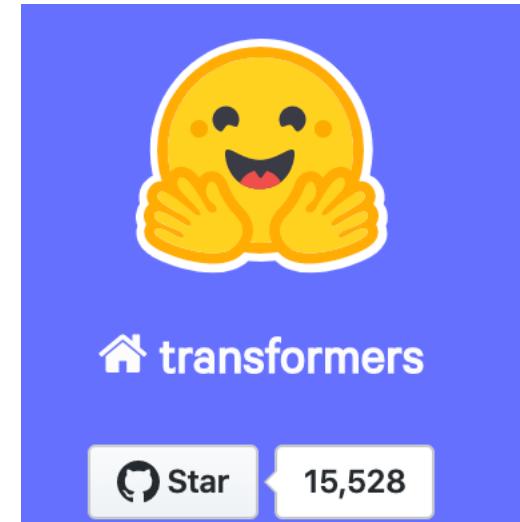
Cat has highest
value.
(dim 763)

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

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

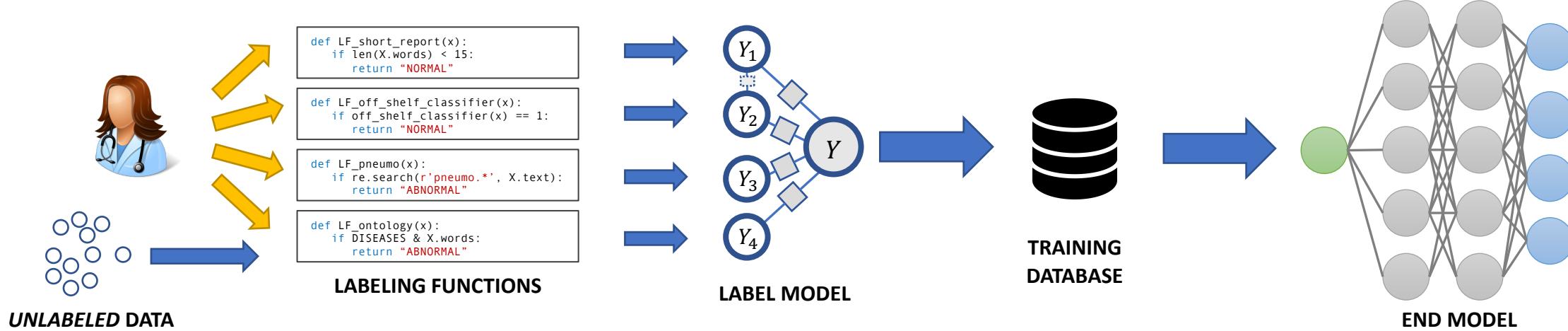
Transfer learning for language

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

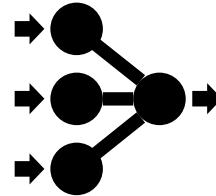


<https://huggingface.co/transformers/>

Weak Supervision Ex: Snorkel



Users write
labeling functions
to heuristically
label data



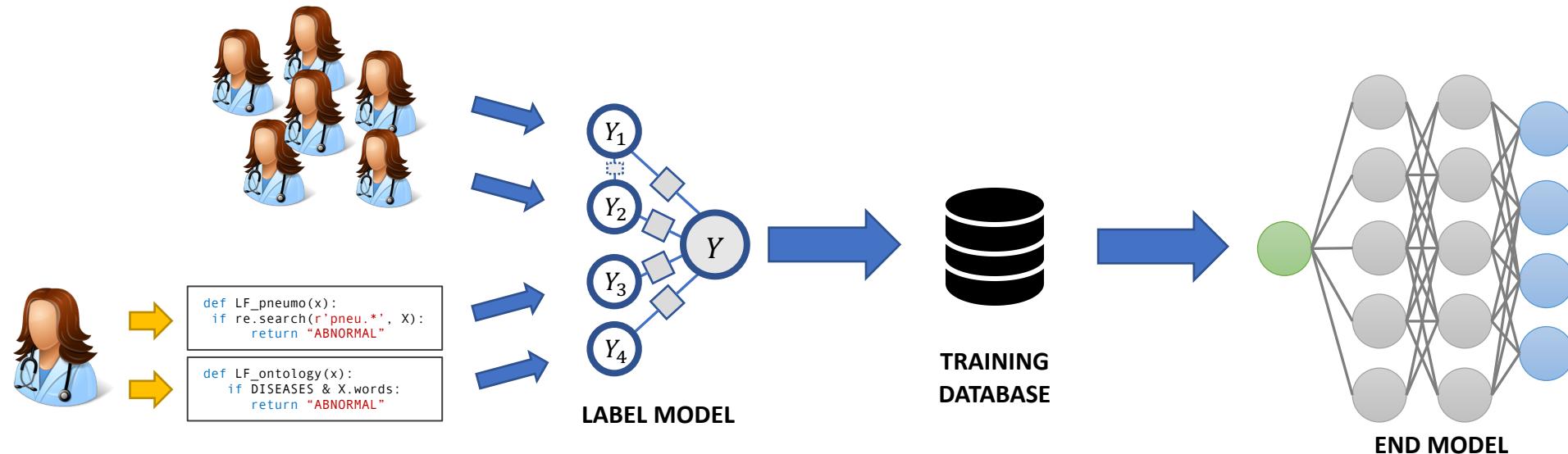
Snorkel
cleans and
combines the
LF labels



The resulting
training database
used to train an
ML model

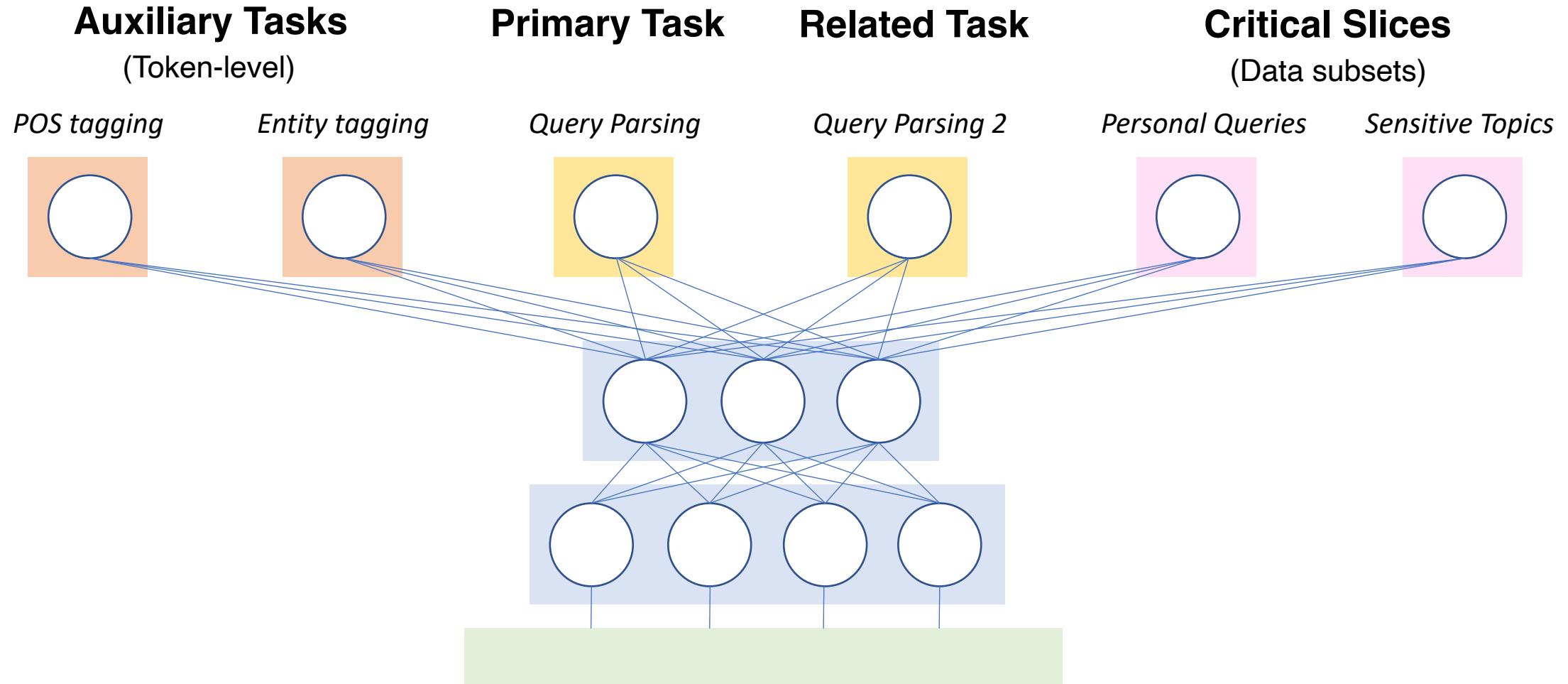
Note: No hand-labeled training data!

Can subsume noisy “crowd” labeling as well



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

Massive Multi-Task Learning (MMTL)

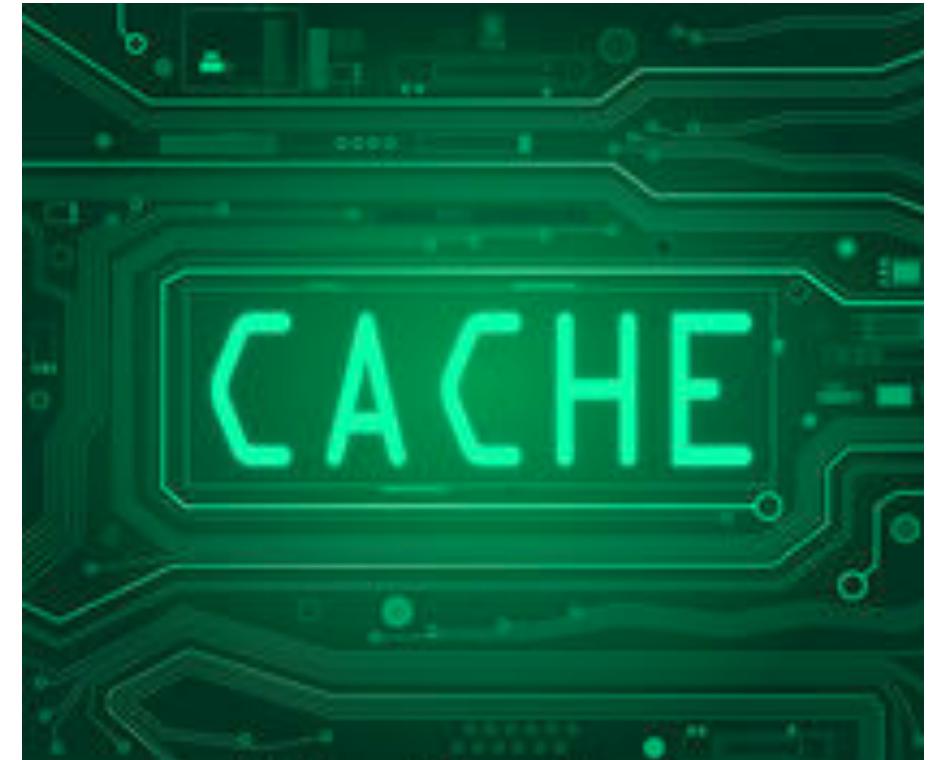


Capitalizing on supervision at every level of granularity

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

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Hidden technical debt.

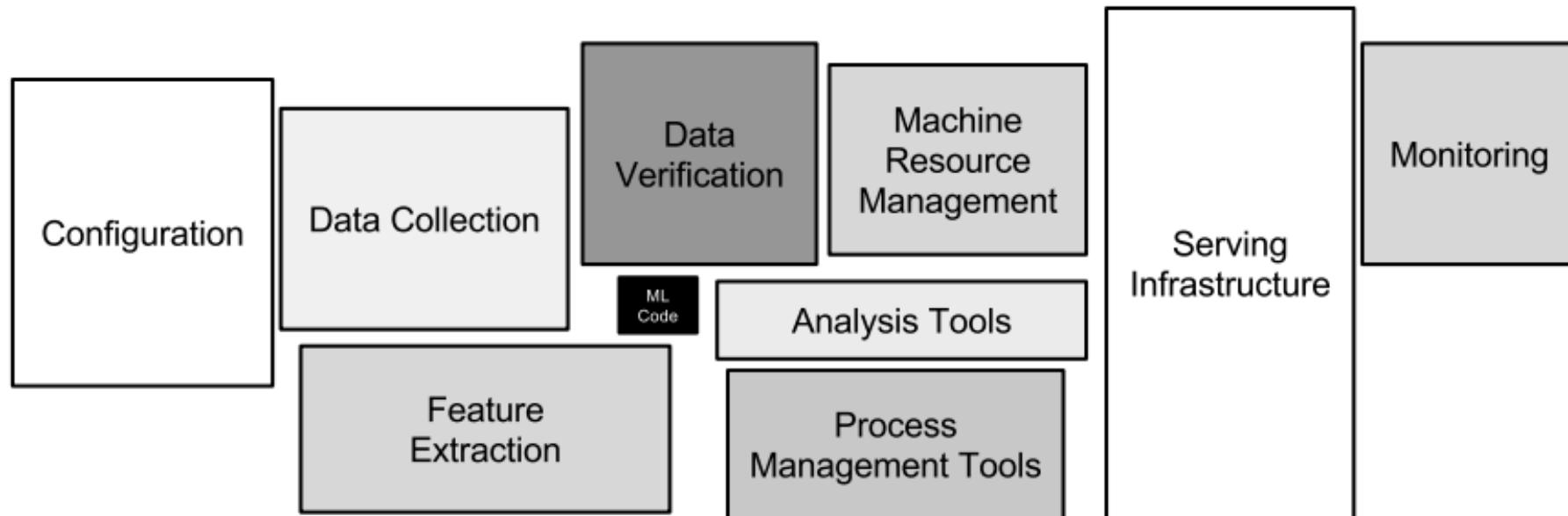


Figure 1: Only a small fraction of real-world ML systems is composed of the ML code, as shown by the small black box in the middle. The required surrounding infrastructure is vast and complex.

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!



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.

HOW NOT TO
BE WRONG



THE POWER *of*
MATHEMATICAL THINKING

JORDAN
ELLENBERG

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*."