Introduction to Deep Learning

9. Environment and Covariate Shift

STAT 157, Spring 2019, UC Berkeley

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courses.d2l.ai/berkeley-stat-157

Training ≠ Testing

- **Generalization performance**
  (the empirical distribution lies)
- **Covariate shift**
  (the covariate distribution lies)
- **Logistic regression**
  (tools to fix shift)
- **Covariate shift correction**
- **Label shift**
  (the label distribution lies)
- **Nonstationary Environments**

$$p_{\text{emp}}(x, y) \neq p(x, y)$$

$$p(x) \neq q(x)$$

$$\log(1 + \exp(-yf(x)))$$

$$\frac{1}{2}\left(p(x)\delta(1, y) + q(x)\delta(-1, y)\right)$$

$$p(y) \neq q(y)$$

aws

Generalization performance

Generalization performance








Generalization performance








Generalization performance









Generalization performance





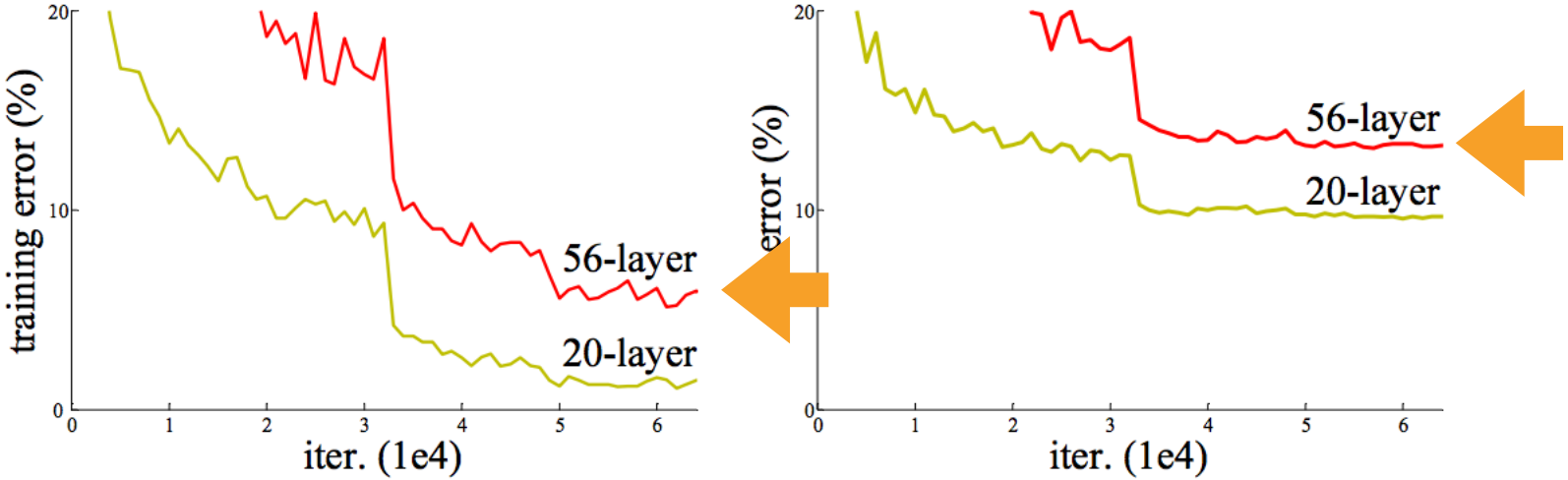




Generalization performance

Only cats and dogs?

- Images, too (e.g. He et al., 2015, ResNet paper)



- Alexa
  (‘Please turn off the coffee machine’ vs. ‘coffee machine off’)

Why?

- Data Distribution p(x,y)
- Dataset drawn from p(x,y)
- Training minimizes empirical risk (plus regularization)

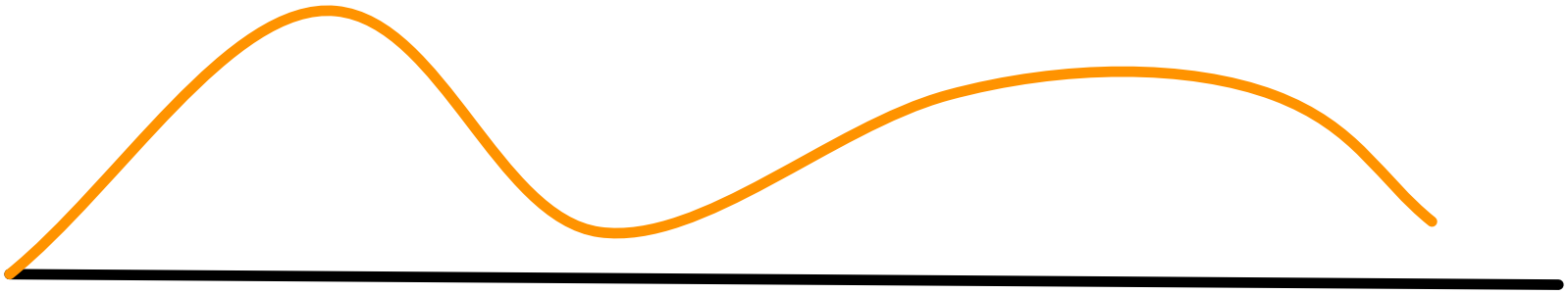
$$\underset{w}{\text{minimize}} \frac{1}{m} \sum_{I=1}^{m} l(f(x_i, w), y_i)$$

- At test time expected risk matters
  (all the other data we could have seen)

$$\mathbf{E}_{(x,y)\sim p} \left[l(f(x, w), y) \right]$$

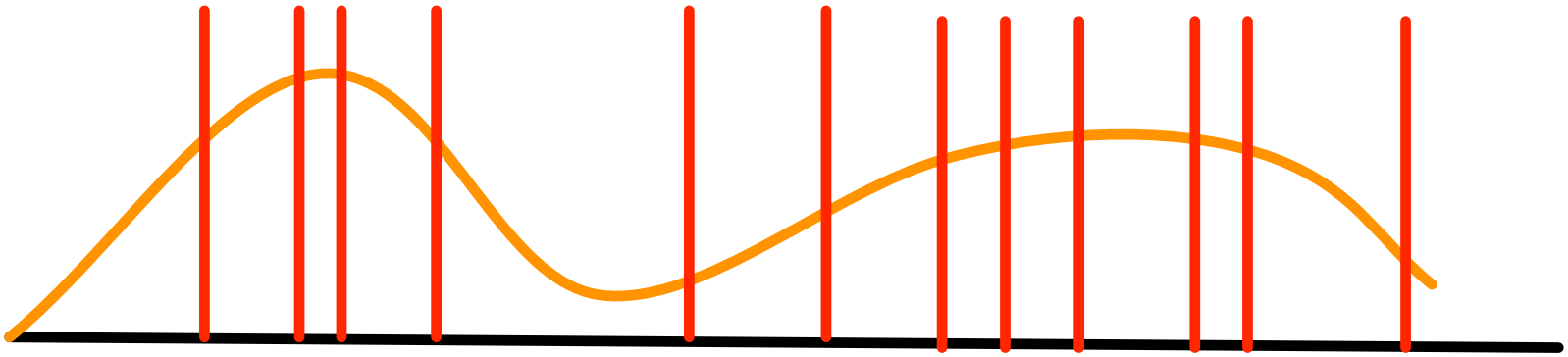
Why

Data Distribution



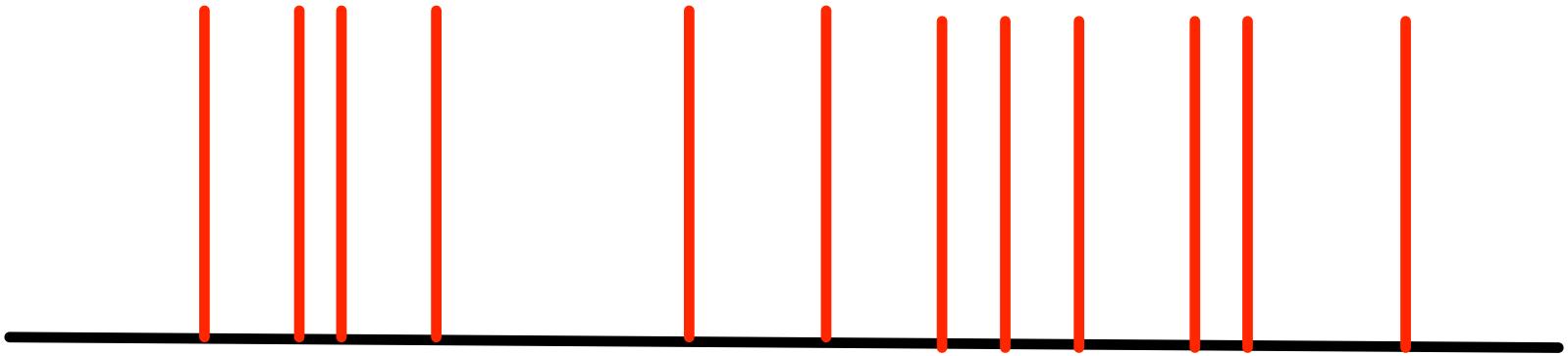
Why

Data Distribution with Empirical Sample



Why

Empirical Sample



Fixing it

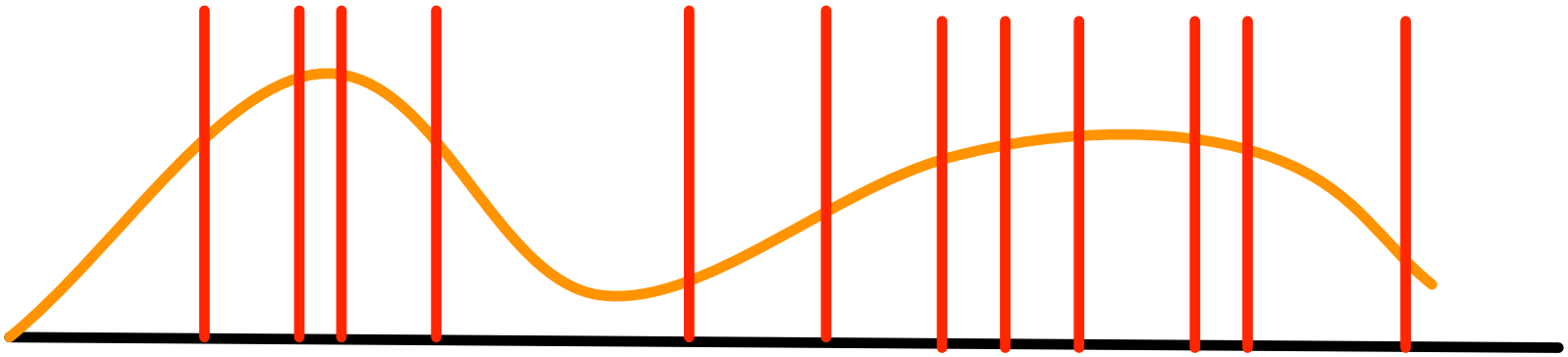
- **Validation set**
  (hold out **separate** data that is not used for training)
- **Chernoff bound**

$$\Pr\left\{\frac{1}{m}\sum_{I=1}^{m} l(f(x_i), y_i)) - \mathbf{E}\left[l(f(x), y)\right] > \epsilon\right\} \leq \exp\left(-2m\epsilon^2\right)$$

- **Why does it work?**
  - Validation set was never used for training (often violated)
  - Loss bounded within [0,1] (otherwise rescale)

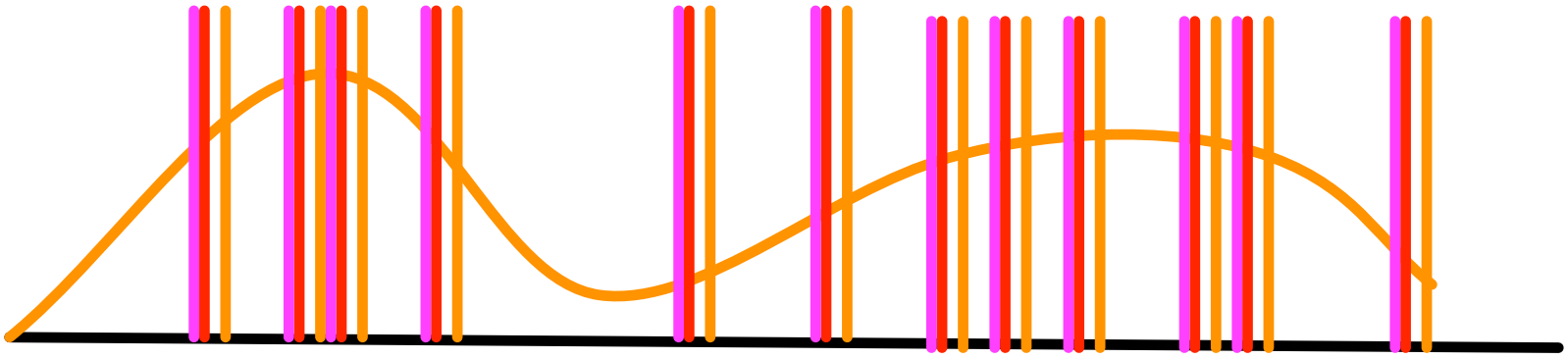
Fixing it

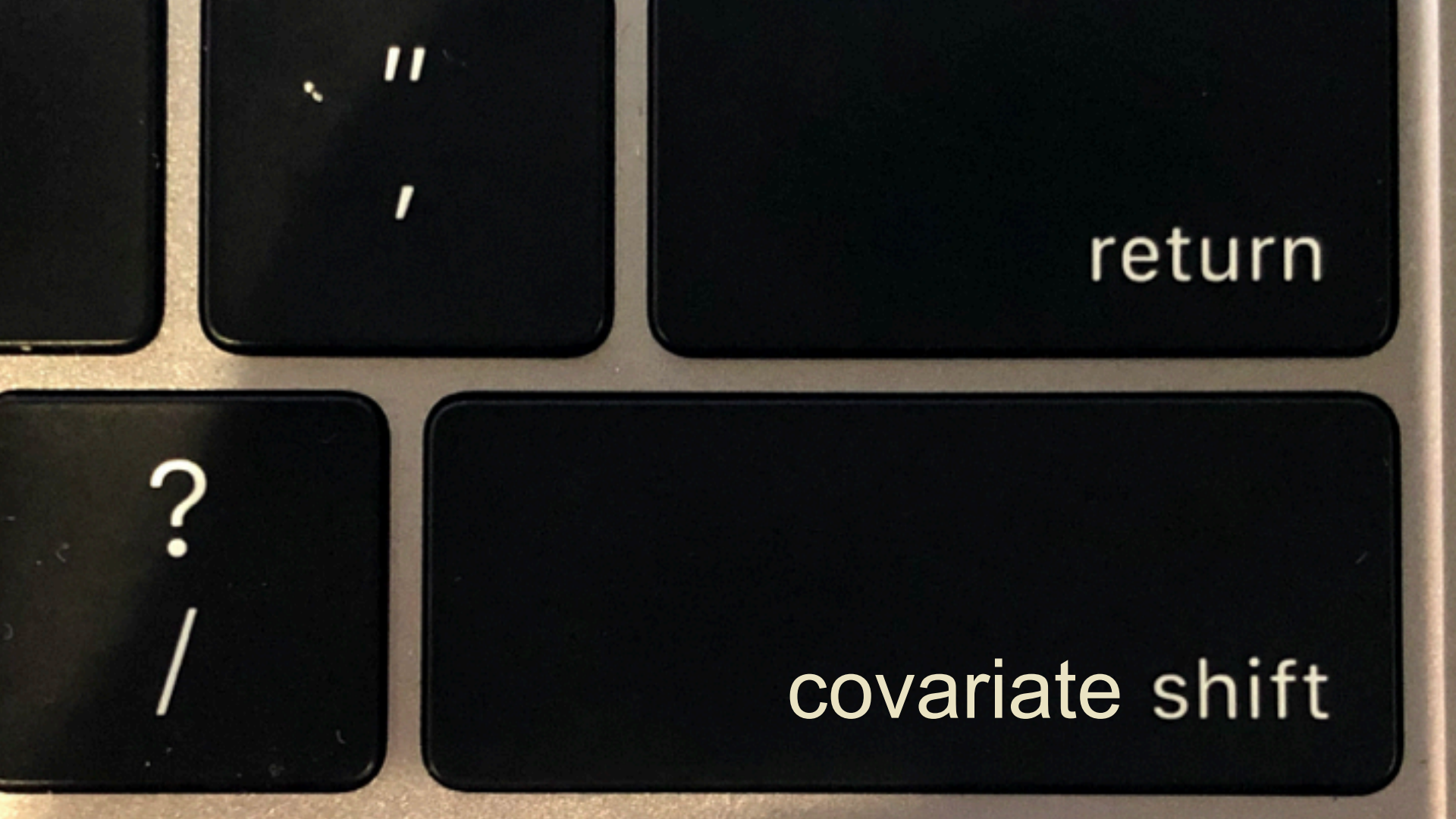
Data Distribution with Empirical Sample



Fixing it

- Input noise (more on this later)
- Dropout (noise within the layers)
- Smoothing the function f (e.g. weight decay)




"
'
return
?
/
covariate shift

Training set








Training set

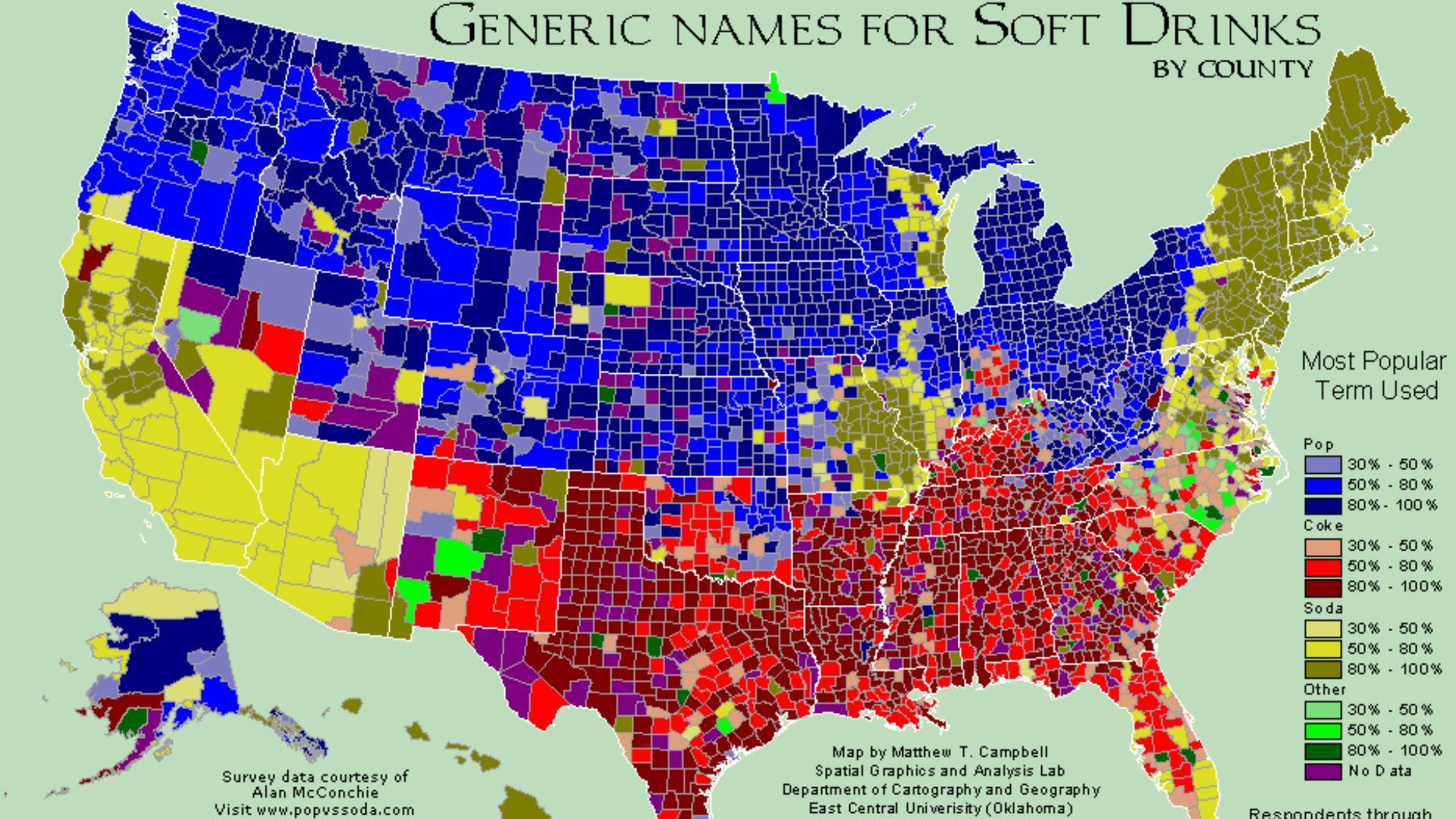
At test time

Why would anyone do this?

Covariate Shift

- **Web search**
  - Training - page relevance data for the US market
  - Testing - recommend pages for Canada (UK, Australia)
- **Speech recognition**
  - Training - West coast accent
  - Testing - Southern drawl, Texan, non-native speaker
- **Language**
  - Training - ‘James, bring me a **soda**’
  - Testing - ‘John, bring me a ‘**pop**’ (or coke, etc.)

Generic names for Soft Drinks
by county



Covariate Shift

- **Medical**
  - Training - University students + old men with prostate cancer
  - Testing - Potentially sick old men
- **Reinforcement Learning**
  - Training - Data gathered with current policy
  - Testing - Environment reacting to updated policy
- **Databases**
  - Training - DB tuned to 2017 usage pattern
  - Testing - DB deployed on AWS in 2018

What is happening? $q(x, y) = q(x)p(y|x)$

- Training Risk

Training data

$$\underset{w}{\text{minimize}} \int dx\, p(x) \int dy\, p(y|x) l(f(x, w), y)$$

$$\text{or rather} \quad \underset{w}{\text{minimize}} \frac{1}{m} \sum_{I=1}^{m} l(f(x_i, w), y_i)$$

- Test Risk is different

Test data

$$\int dx\, q(x) \int dy\, p(y|x) l(f(x, w), y)$$

Fixing it (covariate shift correction)

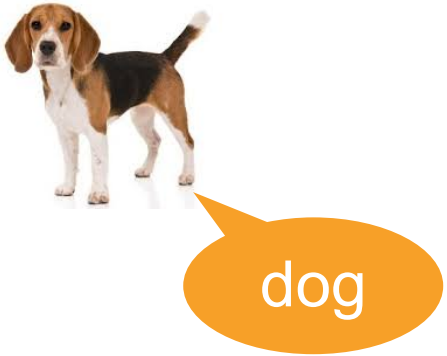
- Basic algebra

$$\int dx\, q(x) f(x) = \int dx\, p(x) \underbrace{\frac{q(x)}{p(x)}}_{\alpha(x)} f(x) = \int dx\, p(x) \alpha(x) f(x)$$

- Need to find density ratio, but we don't have either one.
- Estimating p and q directly is really hard and requires specialized tools. Can we recycle classifiers?

Fairness and Bias
(covariate shift in action & news)

Training set

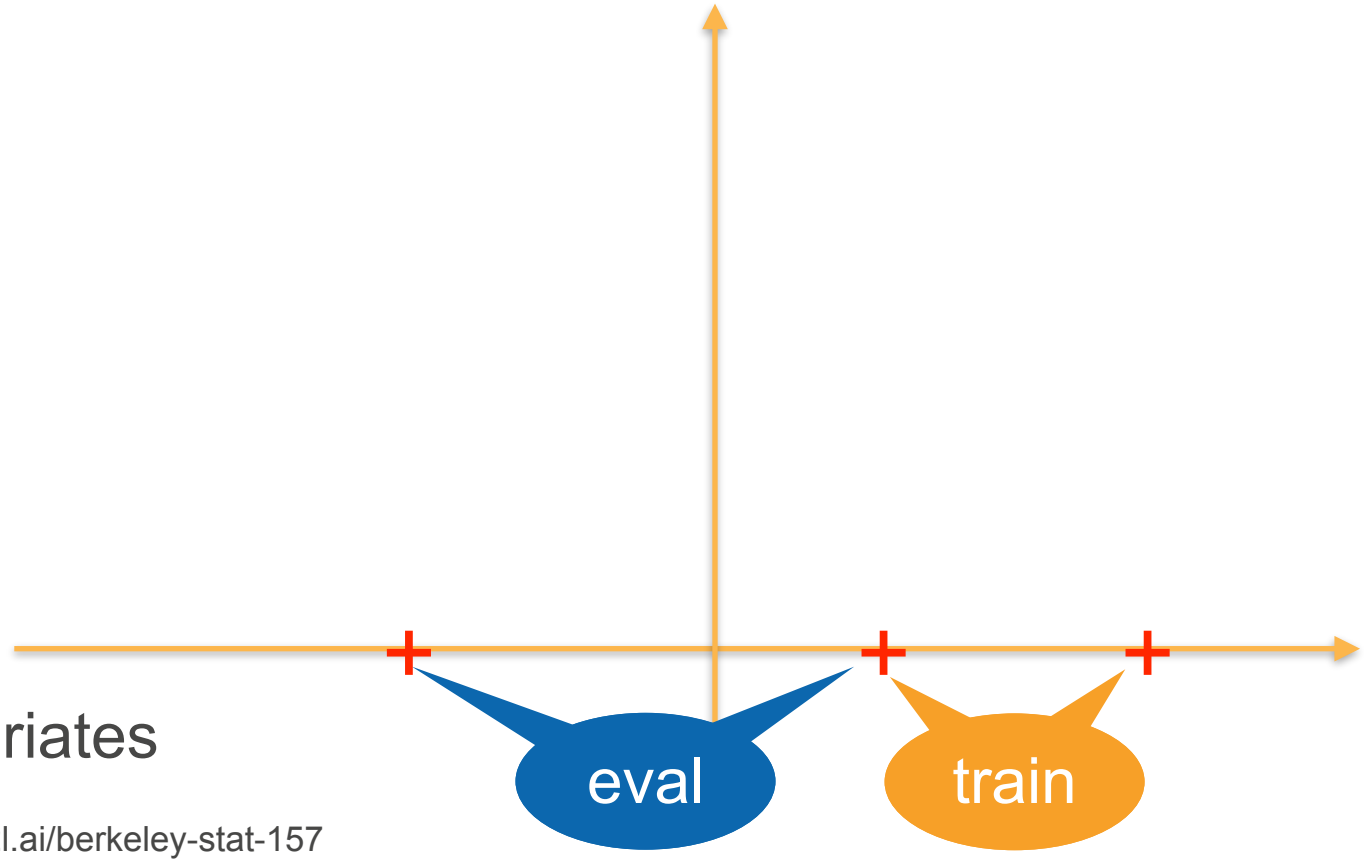


Test set

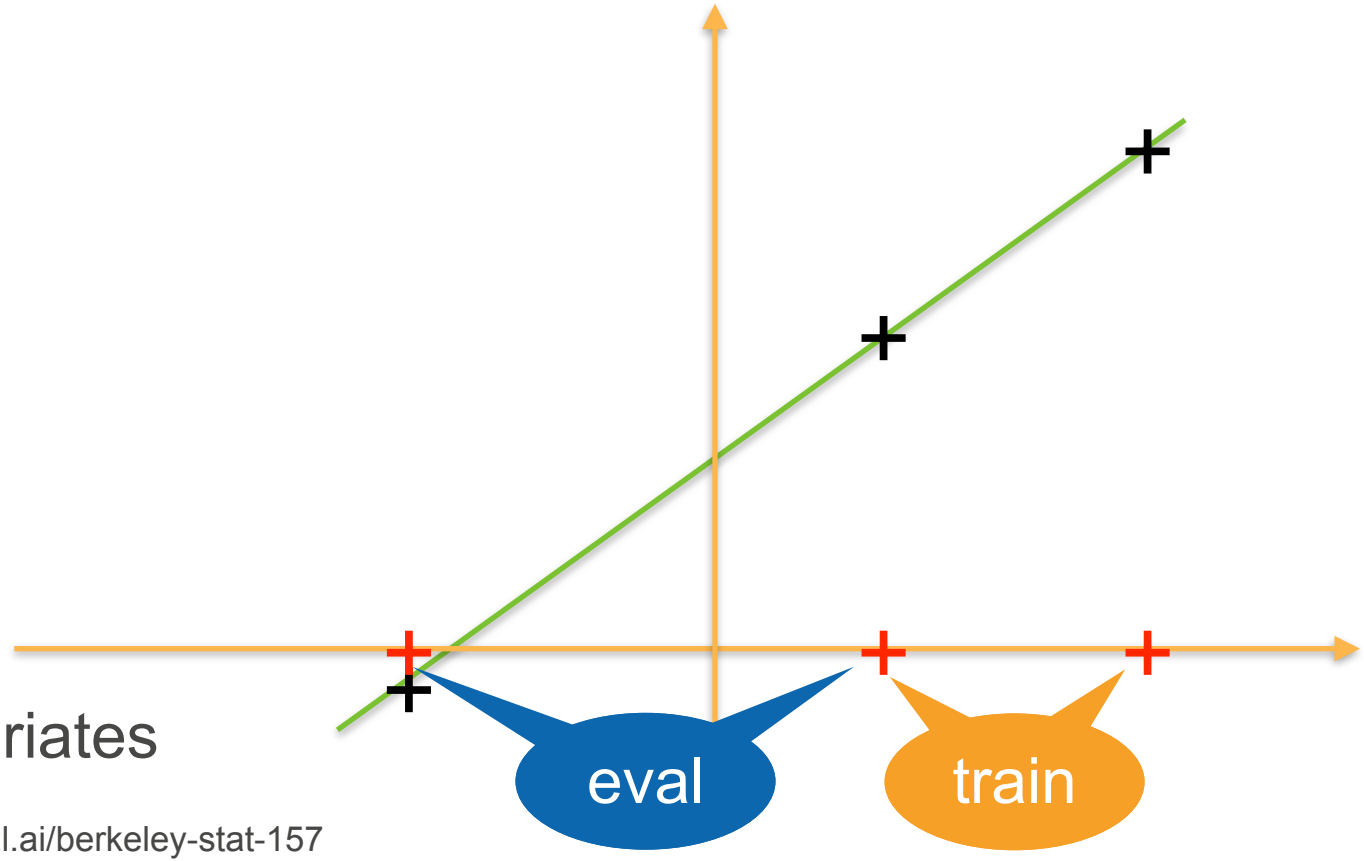
The classifier might perform a lot worse during test time

Why?

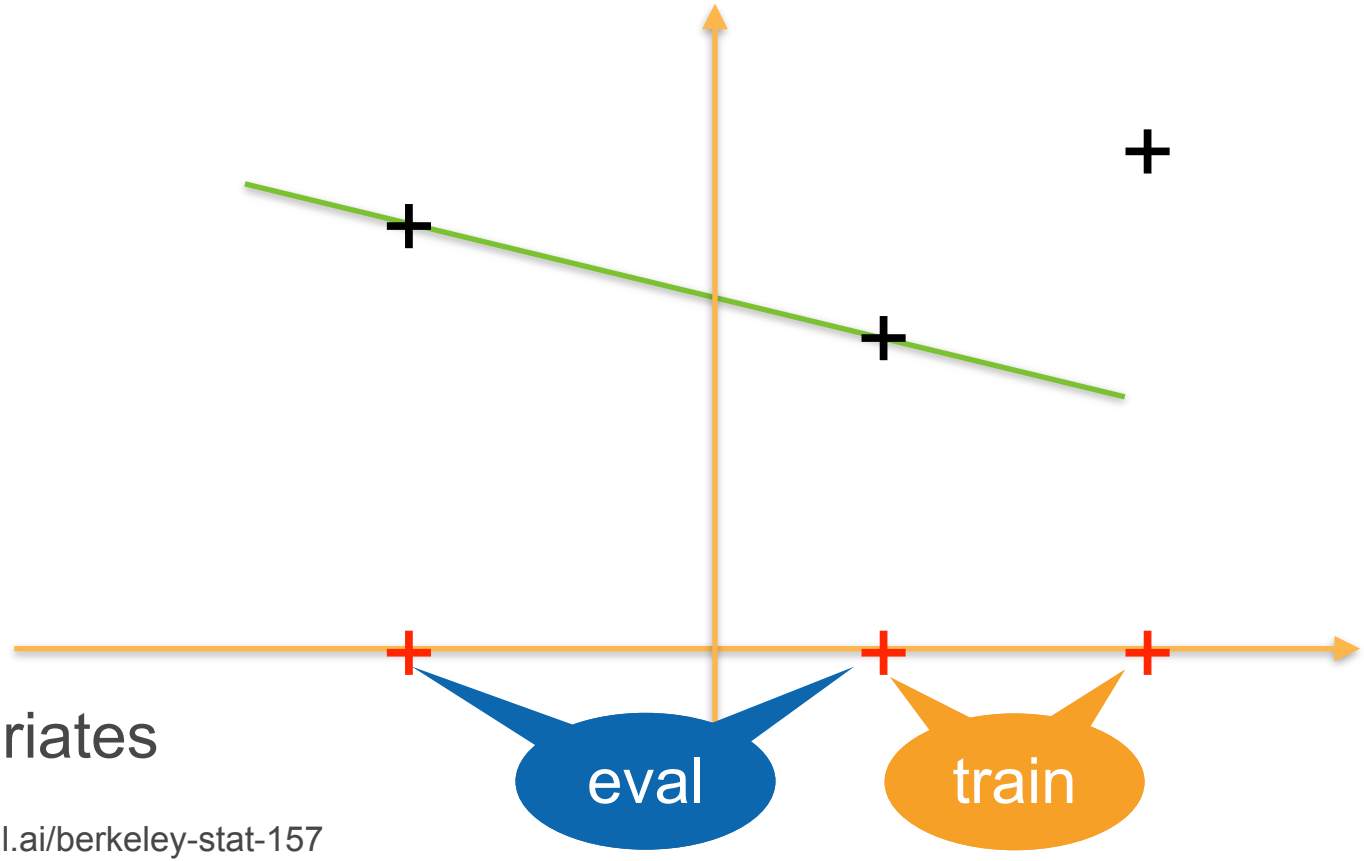
Simple regression problem



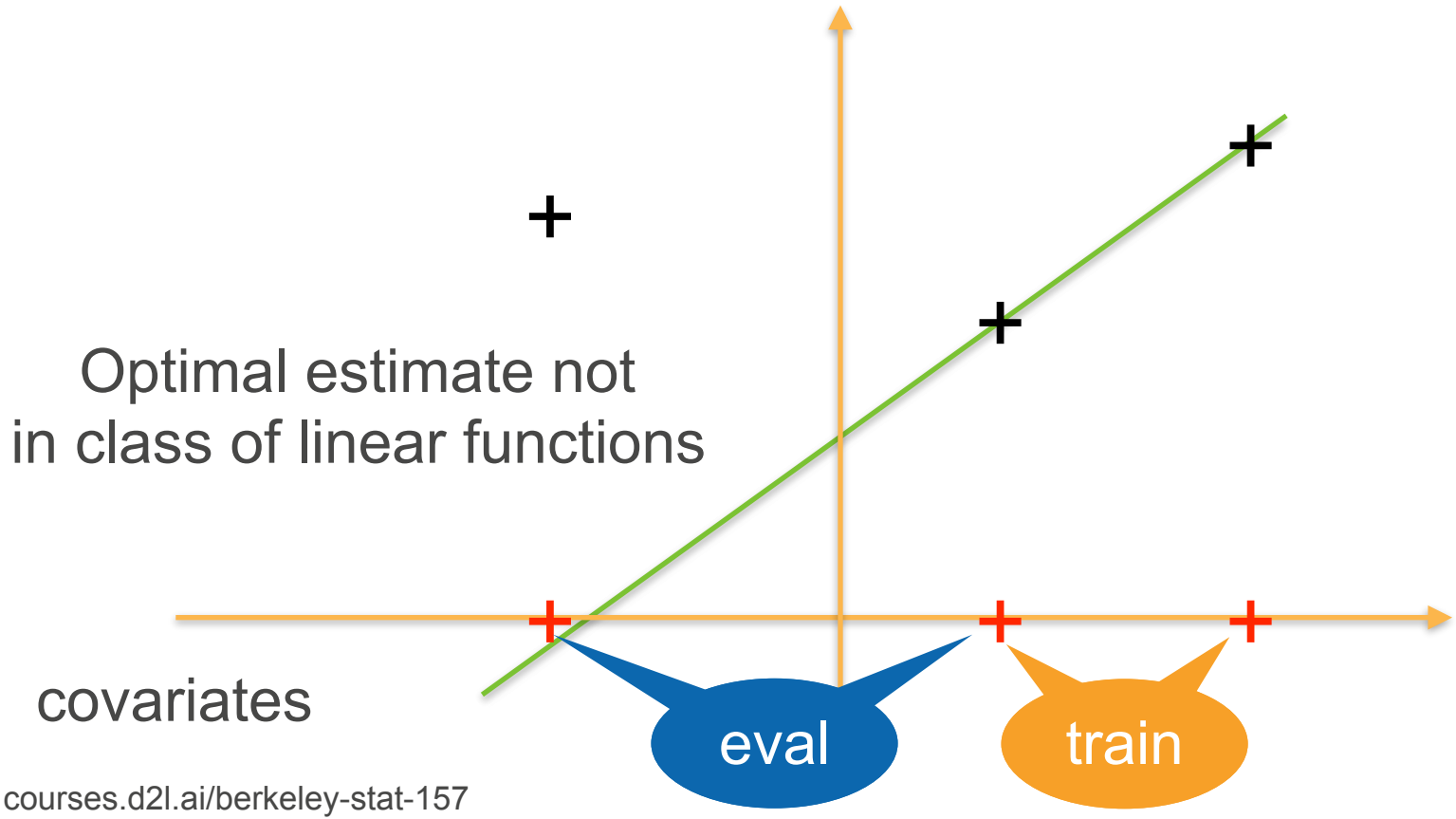
Simple regression problem



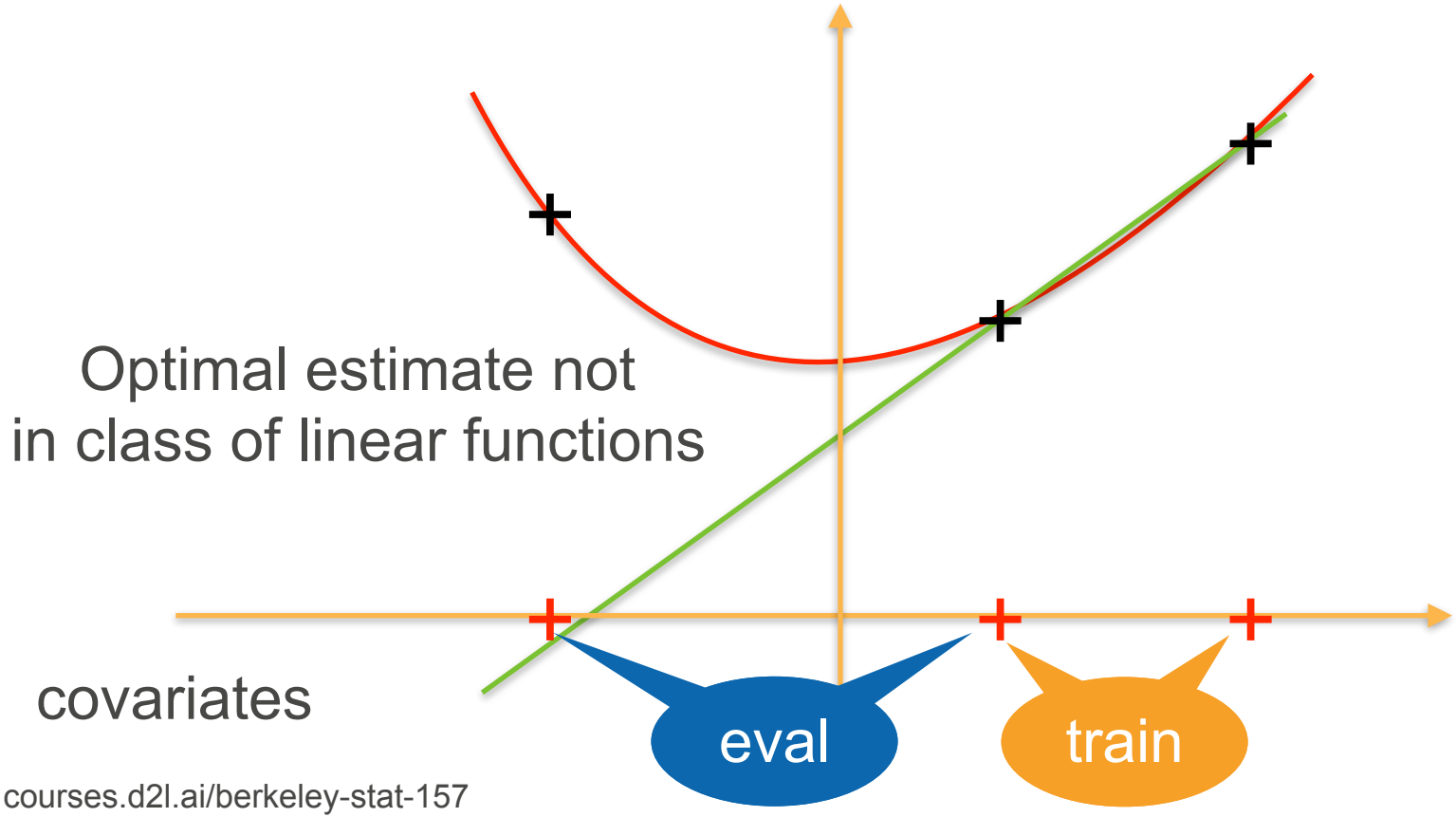
Simple regression problem



Simple regression problem



Simple regression problem



Training error may be misleading (e.g. faces)

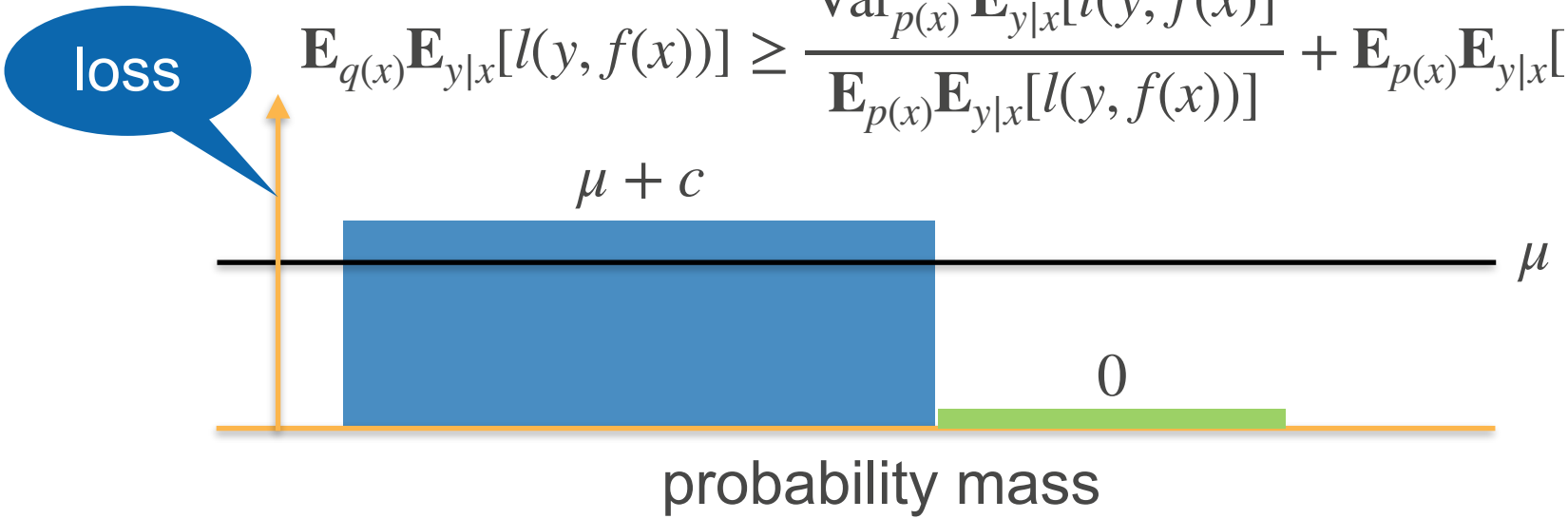
Train on IMDB

Test on weird prof

No Protection against Bias Theorem

- Estimator performs better (or worse) on some data
- We can always find a distribution q that is much worse

$$\mathbf{E}_{q(x)}\mathbf{E}_{y|x}[l(y, f(x))] \geq \frac{\mathrm{Var}_{p(x)}\,\mathbf{E}_{y|x}[l(y, f(x)]}{\mathbf{E}_{p(x)}\mathbf{E}_{y|x}[l(y, f(x))]} + \mathbf{E}_{p(x)}\mathbf{E}_{y|x}[l(y, f(x))]$$



TL;DR Testing where we have insufficient amounts of training data *may* yield strange results.


LOGISTIC
REGRESSION

Recall - Multiclass Classification

Calibrated Scale

- Output matches probabilities (nonnegative, sums to 1)

$$p(y \mid o) = \text{softmax}(o)$$

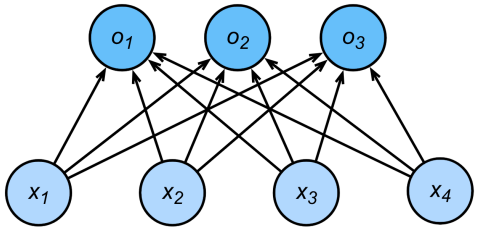
$$= \frac{\exp(o_y)}{\sum_i \exp(o_i)}$$

- Negative log-likelihood

$$-\log p(y \mid o) = \log \sum_i \exp(o_i) - o_y$$

Classification

- Multiple classes, typically multiple outputs
- Score *should* reflect confidence …



Two Classes

- Classes 1 and -1

$$p(y = 1 \mid o) = \text{softmax}(o) = \frac{\exp(o_1)}{\exp(o_{-1}) + \exp(o_1)}$$

- Shift invariance $o_i \leftarrow o_i + c$

$$p(y = 1 \mid o) = \frac{\exp(o_1 + c)}{\exp(o_{-1} + c) + \exp(o_1 + c)} = \frac{\exp(o_1)}{\exp(o_{-1}) + \exp(o_1)}$$

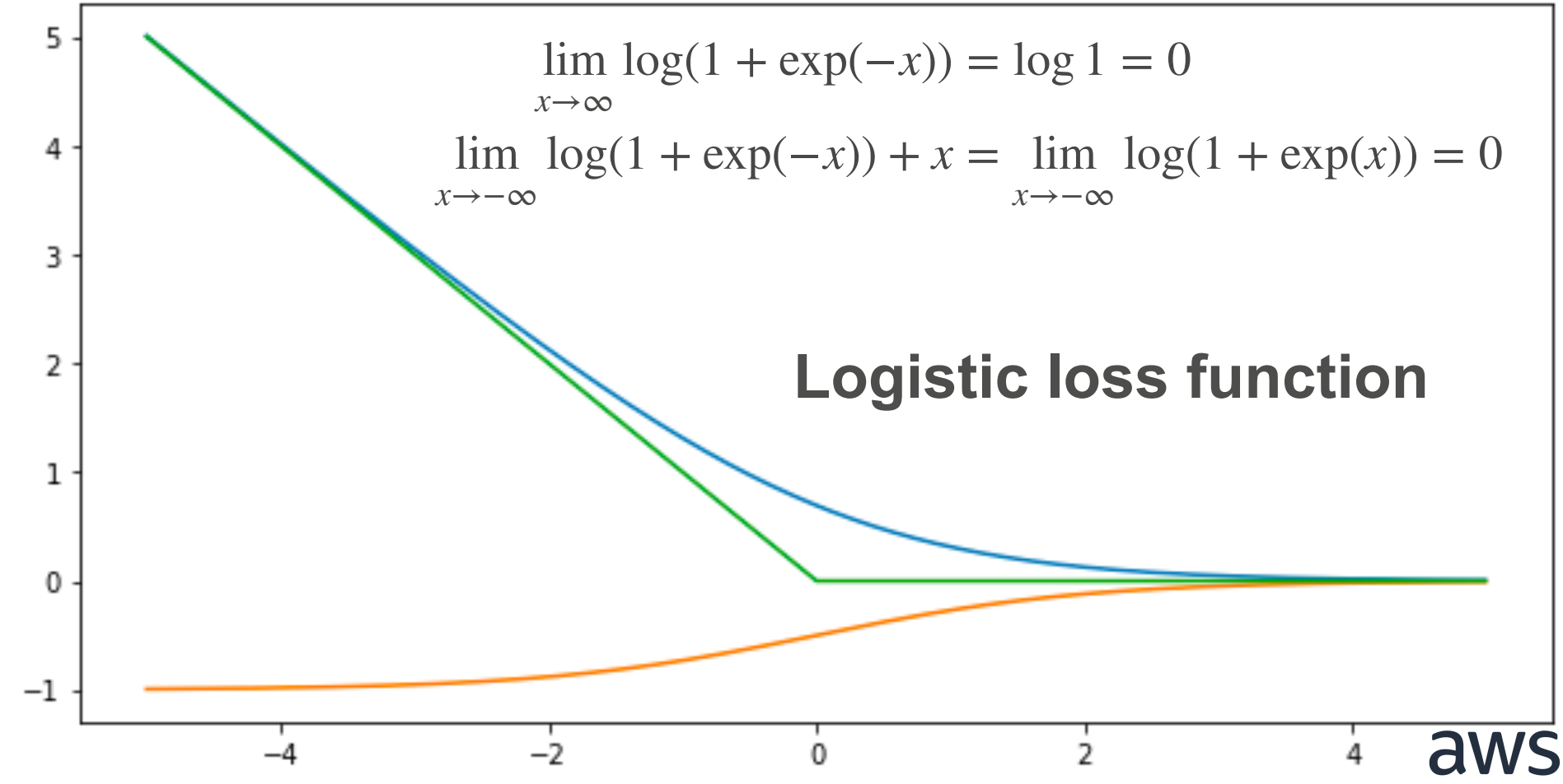
Two Classes

- Choose $o_{\_1} = 0$

$$p(y = 1 \mid o) = \frac{\exp(o_1)}{\exp(0) + \exp(o_1)} = \frac{1}{1 + \exp(-o_1)}$$

- Negative log-likelihood

$$-\log p(y \mid o) = \log(1 + \exp(-yo_1))$$


$\lim_{x \to \infty} \log(1 + \exp(-x)) = \log 1 = 0$
$\lim_{x \to -\infty} \log(1 + \exp(-x)) + x = \lim_{x \to -\infty} \log(1 + \exp(x)) = 0$
Logistic loss function
5
4
3
2
1
0
−1
−4
−2
0
2
4

Logistic Regression Summary

- **Data**

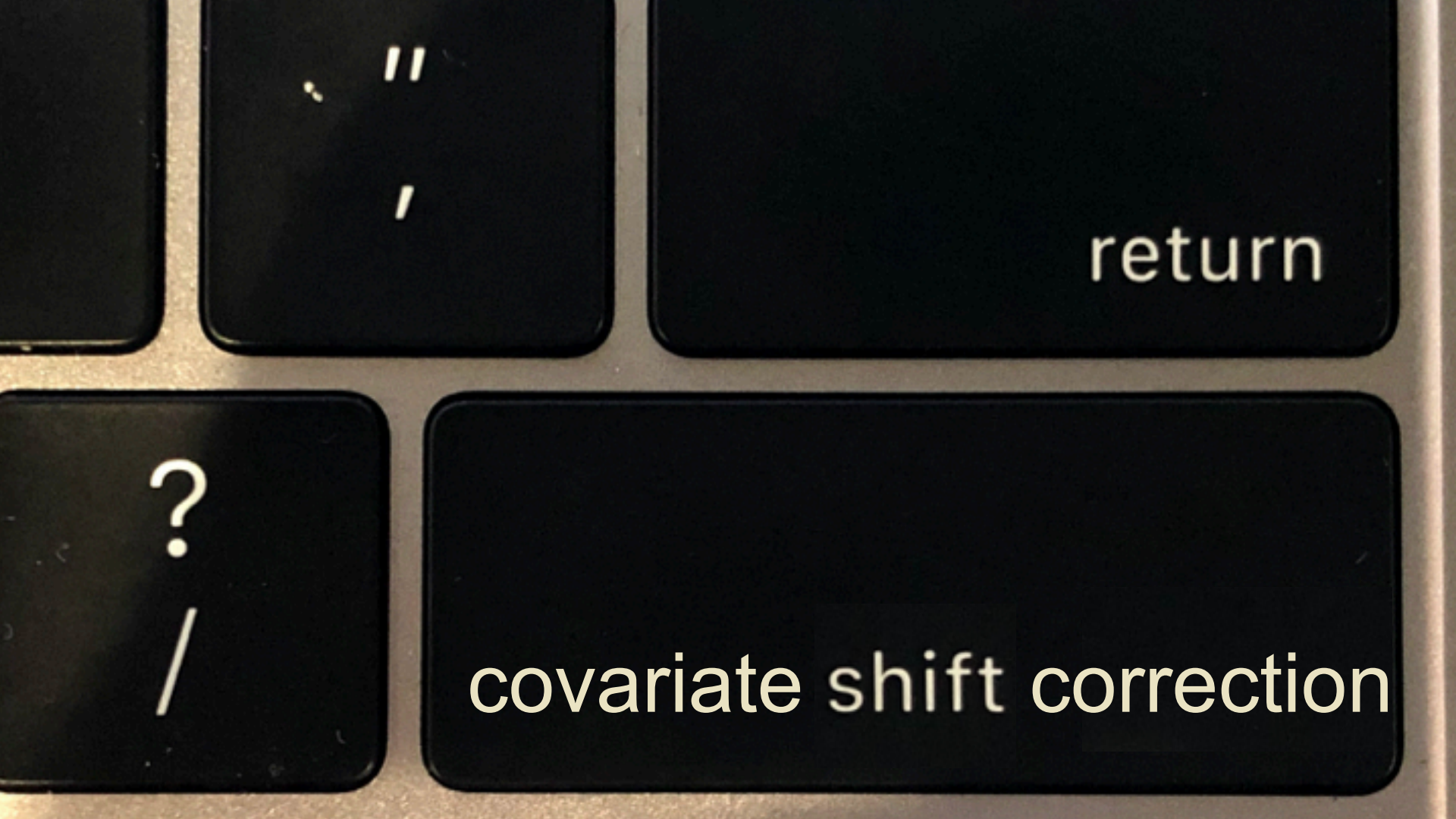
$$(x_i, y_i) \text{ where } x_i \in \mathcal{X} \text{ and } y_i \in \{\pm 1\}$$

- **Objective**

$$\underset{w}{\text{minimize}} - \sum_{i=1}^{m} \log(1 + \exp(-y_i f(x_i, w))) + \text{penalty}(w)$$

- **Conditional Probability Estimate**

$$\log p(y = 1 \mid o) = \frac{1}{1 + \exp(-o)}$$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covariate shift correction

Covariate shift correction

- Propensity scoring

$$\int dx\, q(x) f(x) = \int dx\, p(x) \underbrace{\frac{q(x)}{p(x)}}_{\alpha(x)} f(x) = \int dx\, p(x) \alpha(x) f(x)$$

- Need to find density ratio, but we don't have either one.
- Key idea: train a classifier between p and q

$$r(x, y) = \frac{1}{2}\left[p(x)\delta(y, 1) + q(x)\delta(y, -1)\right]$$

Covariate shift correction

- Conditional class probability

$$r(y=1|x) = \frac{p(x)}{p(x)+q(x)} \text{ and hence } \alpha = \frac{q(x)}{p(x)} = \frac{r(y=-1|x)}{r(y=1|x)}$$

- Logistic regression

$$r(y=1\,|\,x) = \frac{1}{1+\exp(-f(x))}$$

$$\Longrightarrow \alpha(x) = \frac{r(y=-1\,|\,x)}{r(y=1\,|\,x)} = \exp(f(x))$$

Covariate Shift Correction Redux

- Training and test data
- Split **as if it were a binary classification problem** (labels -1 and 1 for training and test respectively)
- Train with **logistic regression** to get f
- Use binary classifier output to reweight data
- Solve original problem but weighted

$$\sum_i l(x_i, y_i, g(x_i, w)) \longrightarrow \sum_i \exp(f(x_i)) \cdot l(x_i, y_i, g(x_i, w))$$

Label shift

Training set








Training set

Test set

Why would anyone do this?

Label Shift

- **Medical diagnosis**
  - Train on data with few sick patients
  - Test on data during flu season where q(flu) > p(flu) while flu symptoms p(symptoms|flu) are still the same
- **Speech recognition**
  - Train on newscast data before election
  - Test on newscast after election (new topics, names, discussions, but still same language)

Label Shift

$$q(x, y) = q(y)p(x|y)$$

- Data generating process p(x|y) is unchanged
- Labels change since the underlying cause changed

- Need to reweight according to $\beta(y) = \frac{q(y)}{p(y)}$ to get

$$\int q(y)\,dy \int p(x|y)\,dx\, l(f(x), y) = \int p(y)\frac{q(y)}{p(y)}\,dy \int p(x|y)\,dx\, l(f(x), y)$$

We don’t have samples from q(y)!

Label Shift $q(x, y) = q(y)p(x|y)$

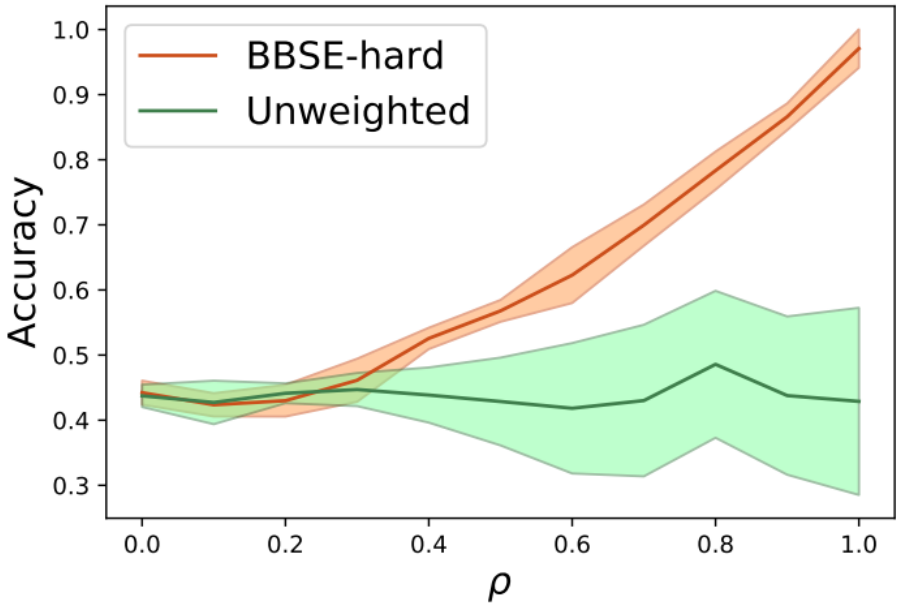
- **Key Idea - measure the estimates on test set**
  - p(x|y) is the same for training and test
  - Distribution of predictions |x,y has to be the same
- **Simple 'spectral' algorithm** (Lipton, Wang, Smola, 2018)
  - Confusion matrix $C[y'|y] = \Pr(\hat{y}(x) = y'|y)$ on hold out
  - Predicted label vector on test set $\mu[y'] = \Pr(\hat{y}(x) = y')$
  - Obtain q(y) via matrix inversion since

$$\mu[y'] = \sum_y C[y'|y]q(y)$$

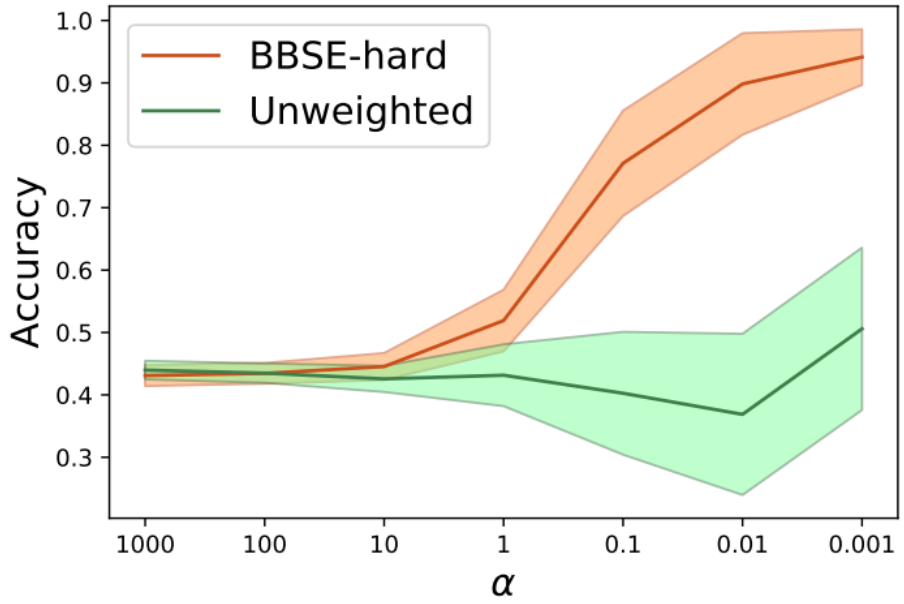
Guarantees

- **Robust under misspecification**
  - Even if the estimates y(x) are wrong, calibration is OK: (same errors on hold-out and test set)
  - Confusion matrix and label vector are concentrated: (use matrix Bernstein inequality)
- **Simple algorithm**
  - Cubic in number of classes, linear in sample size

Black Box Shift Correction on CIFAR10



Tweaking one class probability



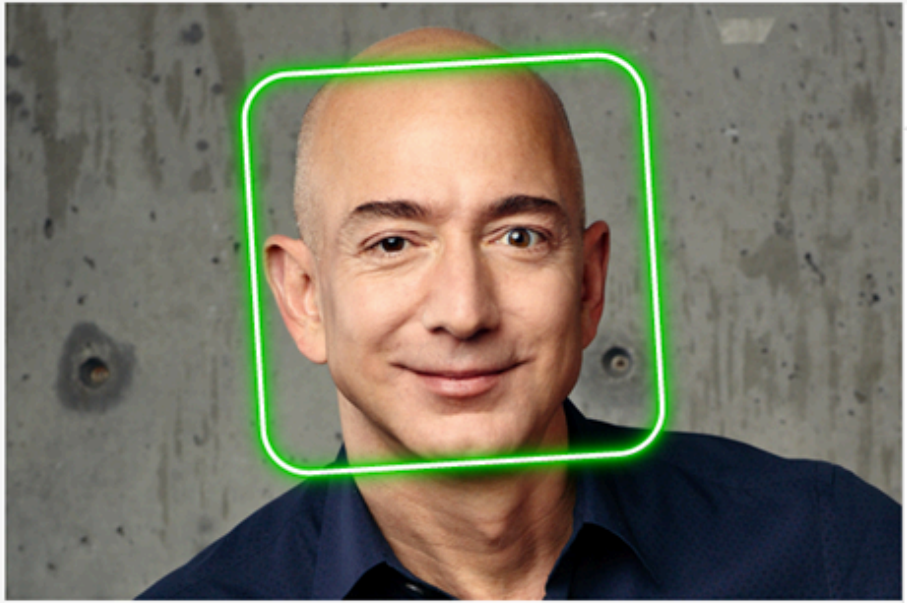
Dirichlet prior over shifts

aws

Adversarial data

Celebrity recognition

Rekognition automatically recognizes celebrities in images and provides confidence scores (Your images aren't stored.)



Done with the demo?
Download SDKs

▼ Results

Jeff Bezos
Learn More

Match confidence 100%

▶ Request

▶ Response

Choose a sample Image

Use your own image

Upload or drag and drop

Use image URL Go

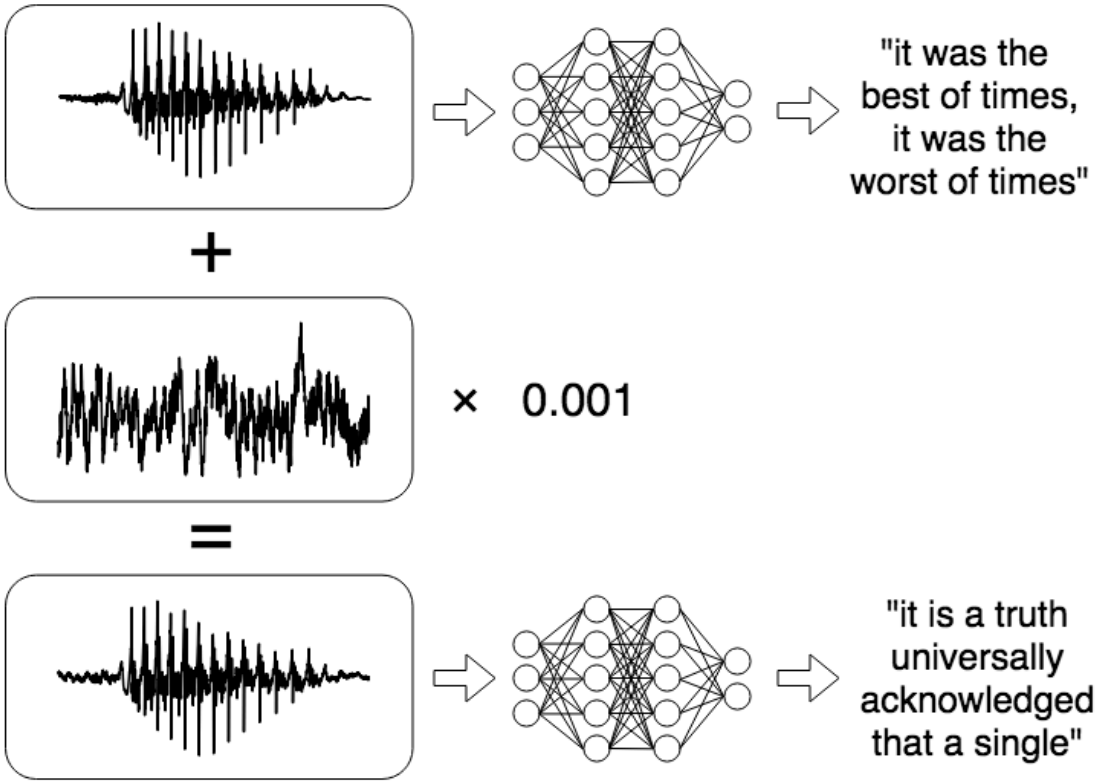
Adversarial Image Generation (e.g. Sharif et al. 2017)

Digital manipulation
to dodge recognition

In real life - via 3D
printed glasses

aws

Adversarial Audio Generation (e.g. Carlini & Wagner, 2018)



- Modify data slightly such as to obtain wrong class

$$\underset{\delta}{\text{maximize}}\ l(f(x+\delta), y)$$

$$\text{subject to } \|\delta\| \leq \epsilon$$

Different norms
Different datasets
Different papers …

aws

Why does this work?

‘Unnatural’ data

- Training and ‘natural’ test data live in small subset
- Adversarial data is slightly off that support
- Function behavior undefined away from where data occurs

‘Unnatural’ data

- Training and ‘natural’ test data live in small subset
- Adversarial data is slightly off that support
- Function behavior undefined away from where data occurs

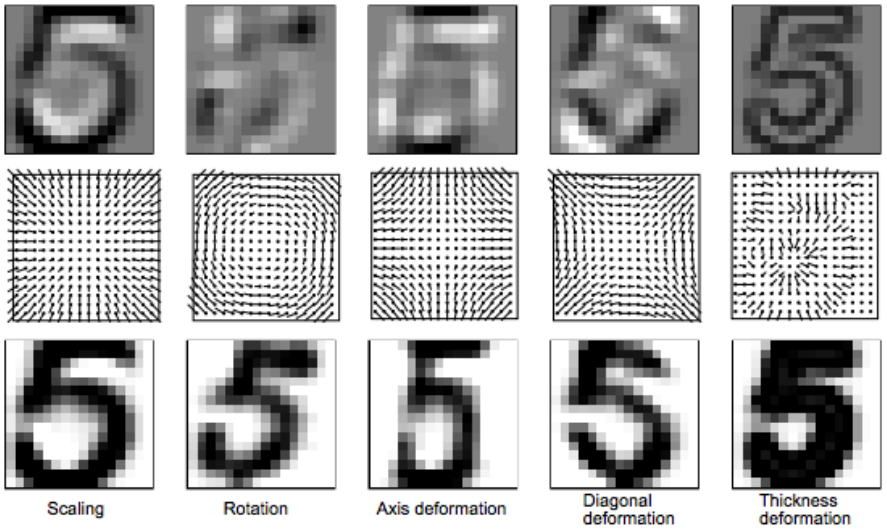
Wow. Breathtaking. Is this new?

Spam defenses

- **While TRUE**
  - Mail host extends dataset and trains new classifier
  - Spammer’s e-mails are rejected
  - Spammer finds a modification that succeeds
- **Examples**
  - Add highly scoring words (or sentences) to email
  - Add highly scoring sentences (and vary them)
  - Change or forge header (‘Dear Alex, …’)

Invariances

- Tangent Distance (Simard et al., 1995)
  - Invariance transforms don’t change the label
  - Explore data and their neighborhood



Invariances

- **Virtual Support Vectors** (Schoelkopf, 1997)
  Only change the data at the boundary (not enough RAM)
- **Data augmentation for training**
  - **Imagenet** (pretty much every paper)
    Cropping, scaling, change mean, per channel, …
  - **Speech Recognition**
    Background noise, scenes, …
  - **Document Analysis**
    Random substrings, word removal, insertion

Invariant and robust loss

- **Convex loss** (Teo et al, 2005)
  - Family of transformations $\delta \in \Delta$
  - Penalty for extreme transformations $1 \geq \eta(\delta) \geq 0$
  - Find the 'worst' possible example at each step

Adversarially Robust Networks

$$L(x, y, f) = \sup_{\delta \in \Delta} \eta(\delta) l(f(x + \delta), y)$$

e.g. adversarial example generator Finds worst possible

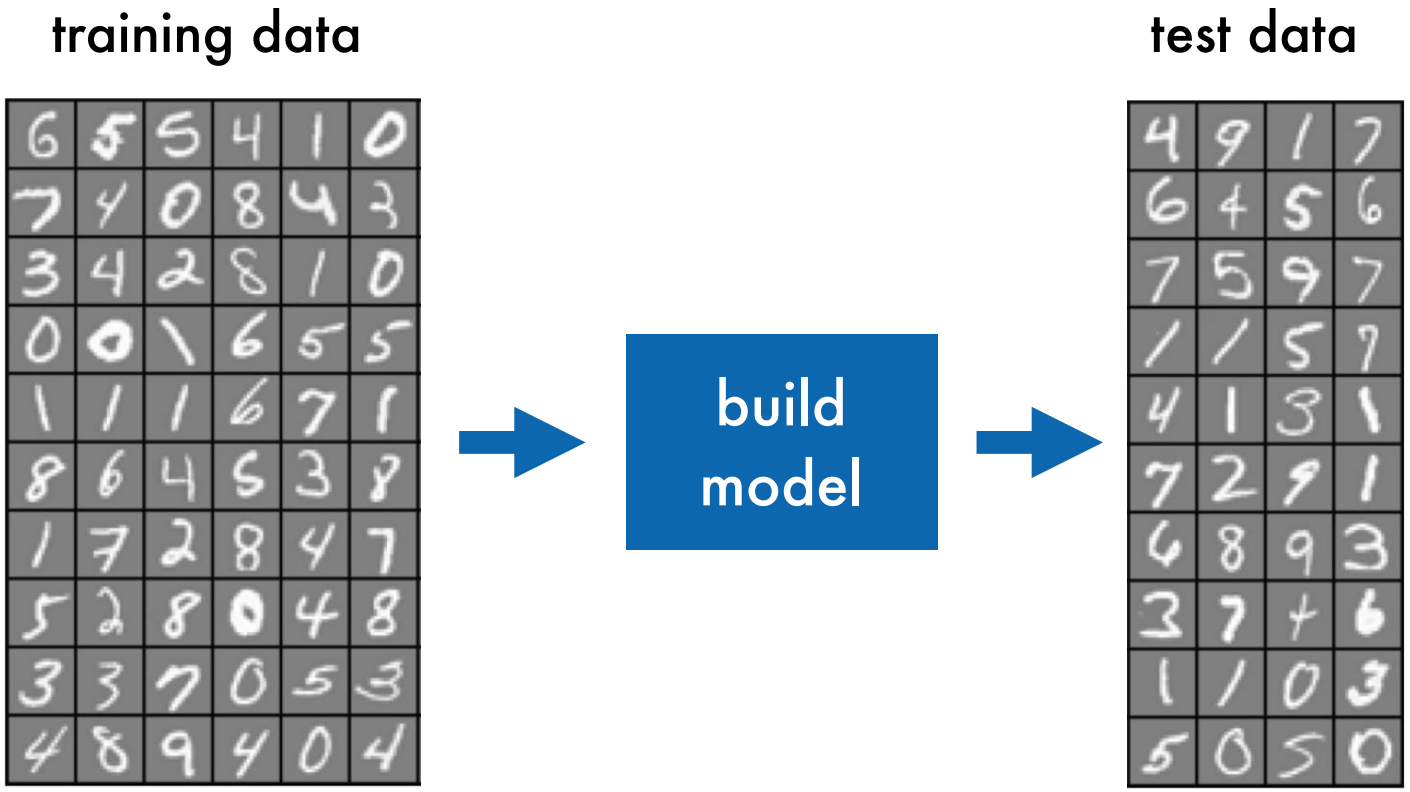
Reduced penalty for extreme distortions

Nonstationary Environments

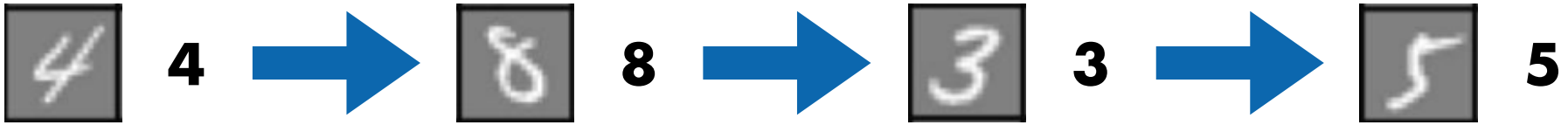
Interaction with Environment

- **Batch** (download a book)
  Observe training data (x_1,y_1) ... (x_l,y_l) then deploy
- **Online** (follow the class)
  Observe x, predict f(x), observe y (stock market, homework)
- **Active learning** (ask questions in class)
  Query y for x, improve model, pick new x
- **Bandits** (do well at homework)
  Pick arm, get reward, pick new arm (also with context)
- **Reinforcement Learning** (play chess, drive a car)
  Take action, environment responds, take new action

Batch



Online



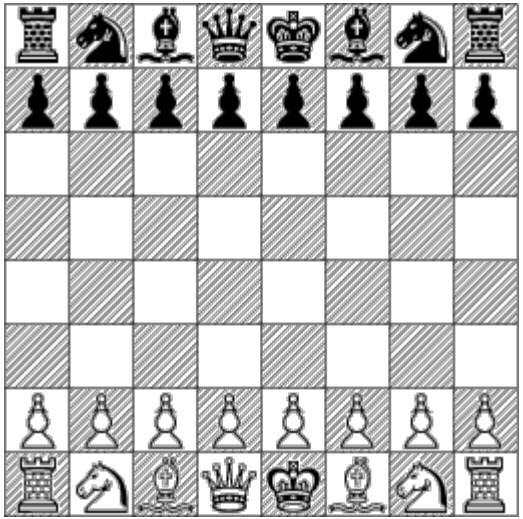
System improves as we see more data

Bandits

- Choose an arm (action)
- See what happens (get reward)
- Update model
- Choose next arm (action)
  The bandit **doesn't remember** what you did last summer.

Stateful Systems

Reinforcement Learning & Control



- Take action
- Environment reacts
- Observe stuff
- Update model

Repeat

- environment (cooperative, adversary, doesn't care)
- memory (goldfish, elephant)
- state space (tic tac toe, chess, car)
- past observations (server log, generated during training)

Reinforcement Learning & Control

- **Games**
  - Chess, Go, Backgammon (fully observed)
  - Poker, Starcraft, ATARI (partially observed, random)
- **Parallelism**
  - Computation advertising, recommender systems (multiple agents & independent parallel games)
  - Load balancing & scheduling (multiple agents)
- **Actions**
  - Continuous decisions (driving, flying, robots in general, HVAC)
  - Discrete (elevator, work allocation)
- **Simulations**
  - MuJoCo style
  - Only reality (server center)

Training ≠ Testing

- **Generalization performance**
  (the empirical distribution lies)
- **Covariate shift**
  (the covariate distribution lies)
- **Logistic regression**
  (tools to fix shift)
- **Covariate shift correction**
- **Label shift**
  (the label distribution lies)
- **Nonstationary Environments**

$$p_{\text{emp}}(x, y) \neq p(x, y)$$

$$p(x) \neq q(x)$$

$$\log(1 + \exp(-yf(x)))$$

$$\frac{1}{2}\left(p(x)\delta(1, y) + q(x)\delta(-1, y)\right)$$

$$p(y) \neq q(y)$$

aws