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**

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

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

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

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

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

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Generalization performance

Generalization performance








Generalization performance








Generalization performance









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Generalization performance





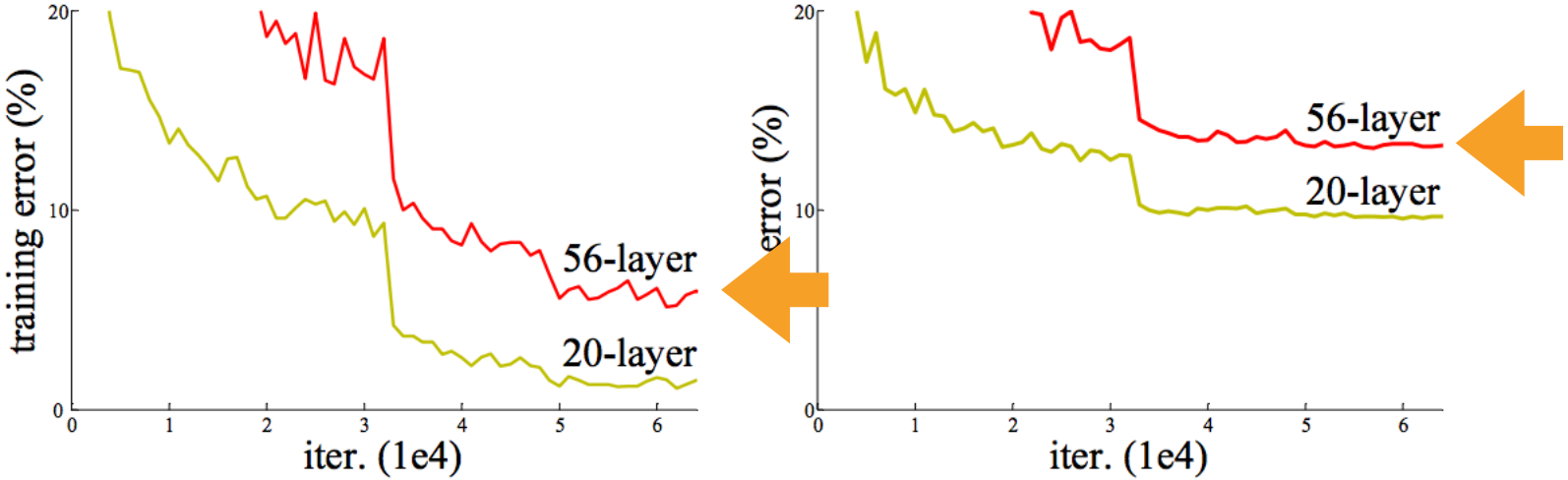




Generalization performance

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)

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

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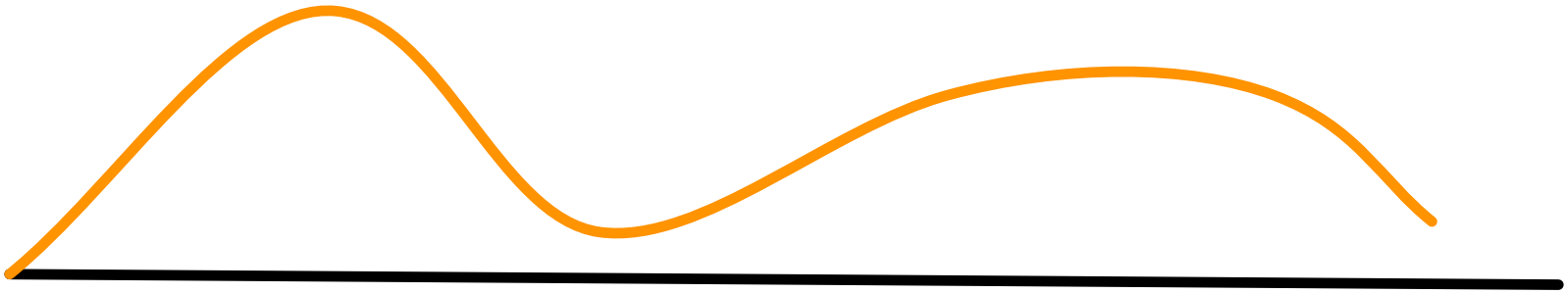
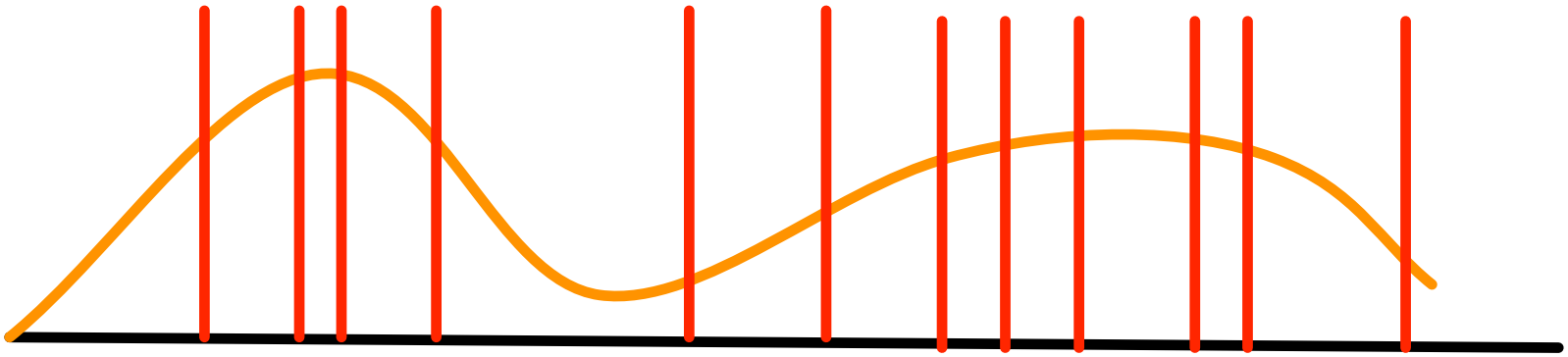
Why

Data Distribution



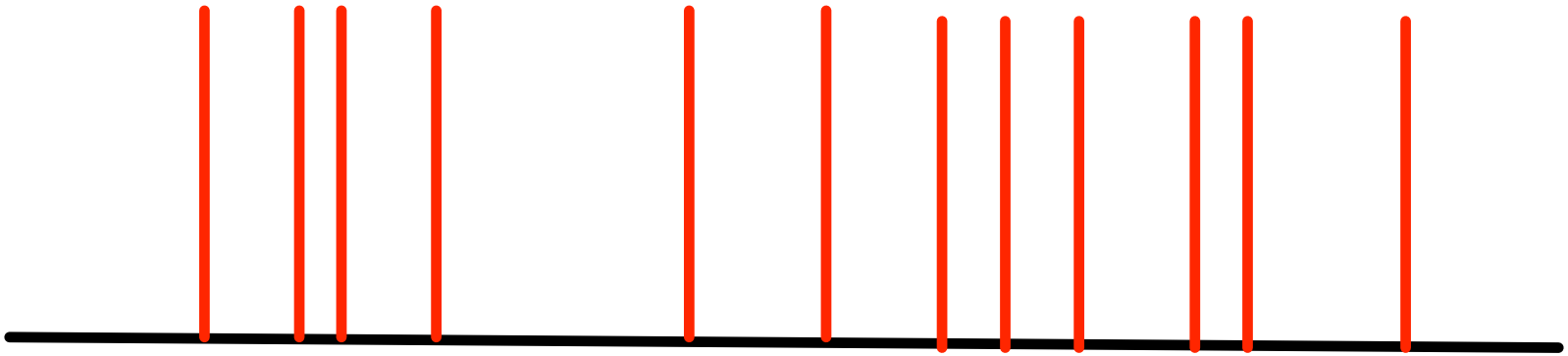
Why

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)

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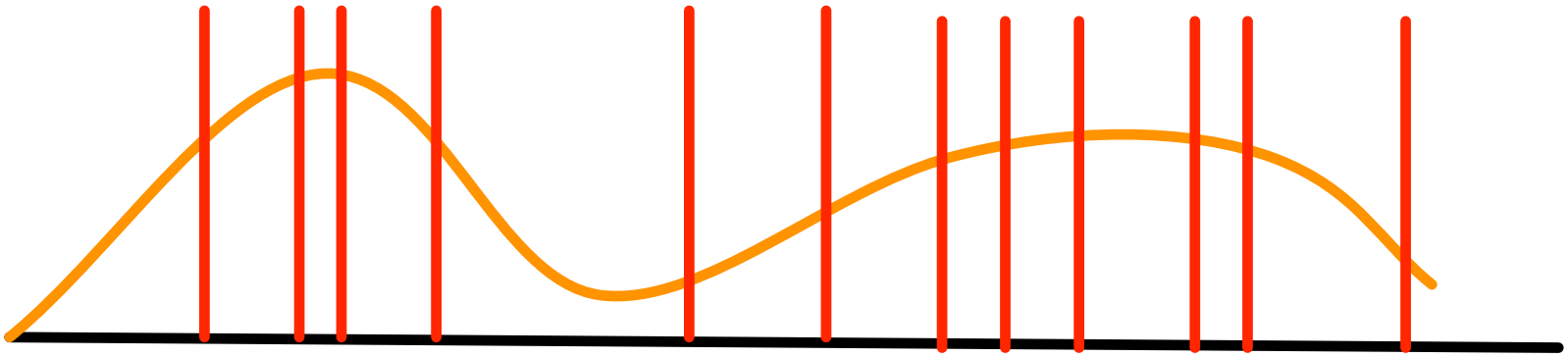
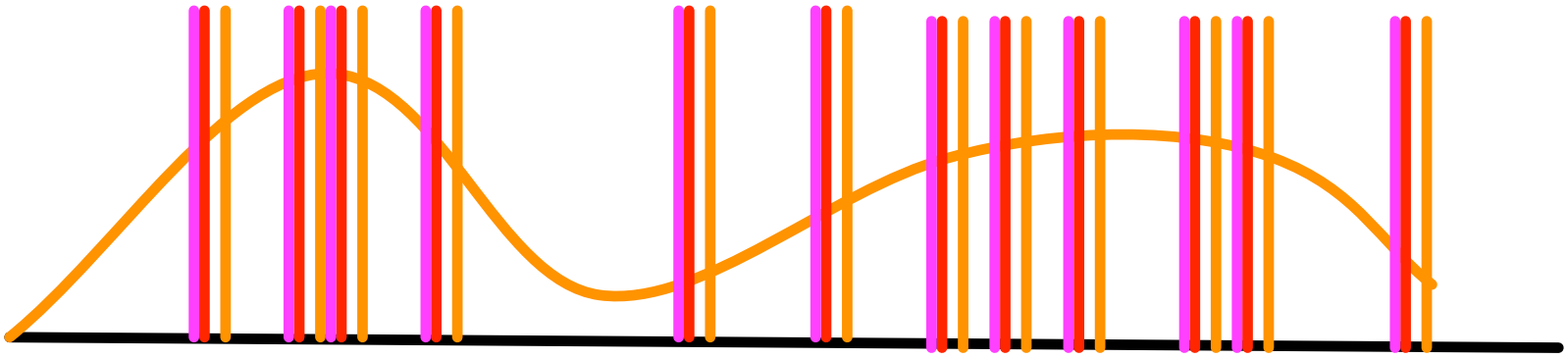
Fixing it

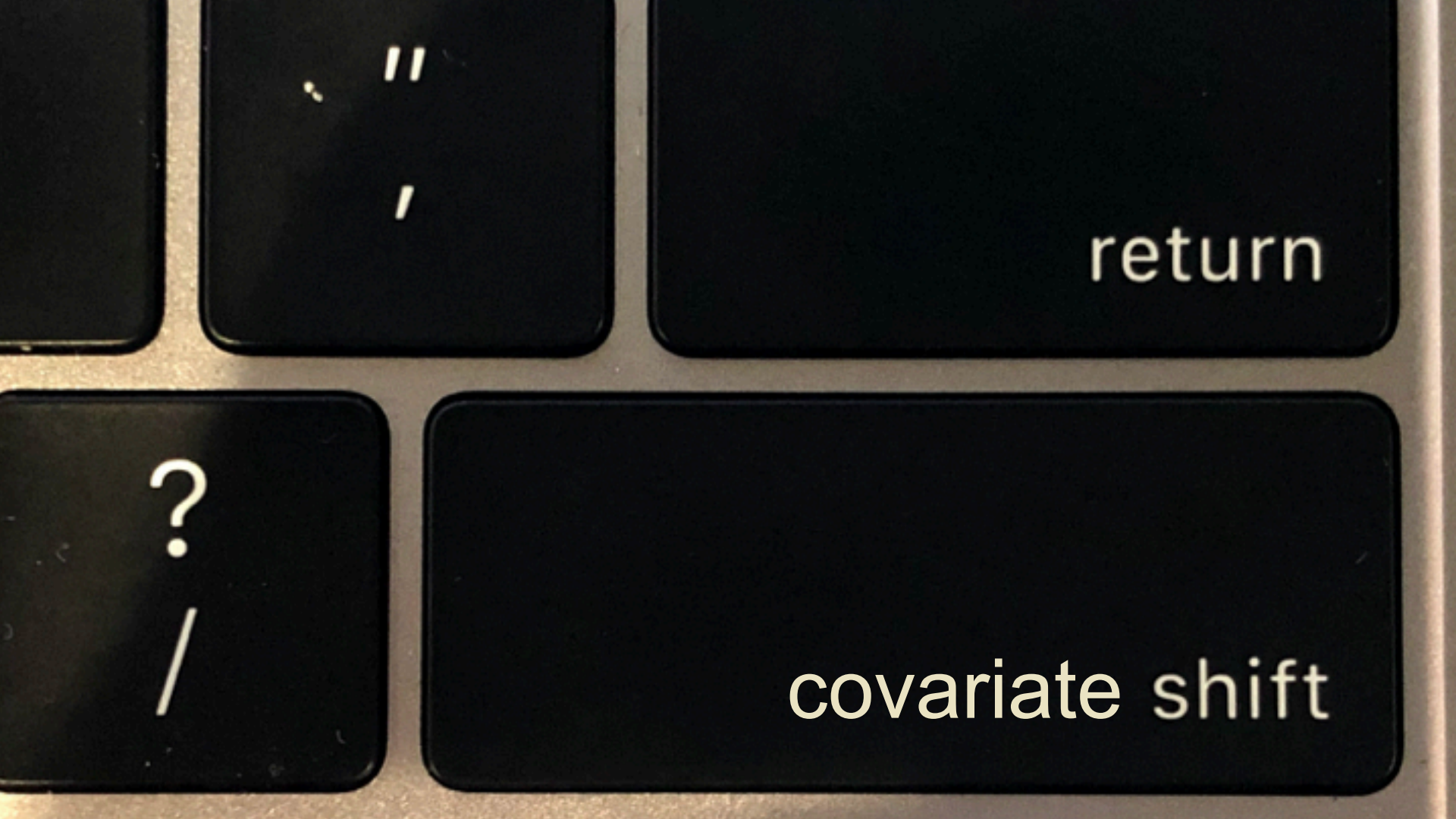
Data Distribution with Empirical Sample



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.)

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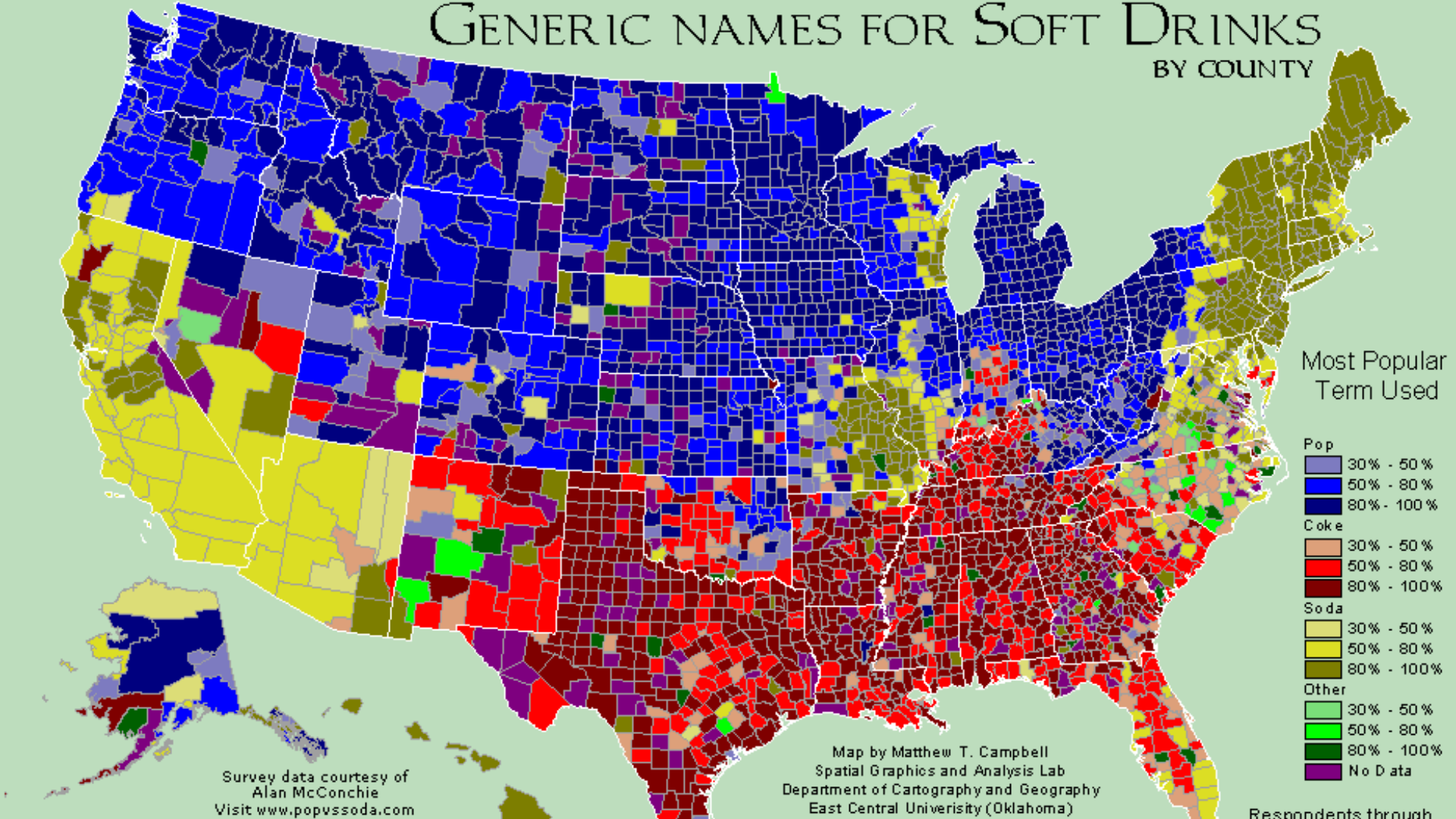
Generic names for Soft Drinks
by county



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

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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

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

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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?

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Fairness and Bias
(covariate shift in action & news)

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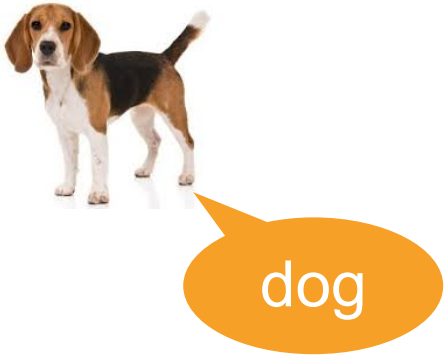
Training set



Test set

The classifier might perform a lot worse during test time

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Why?

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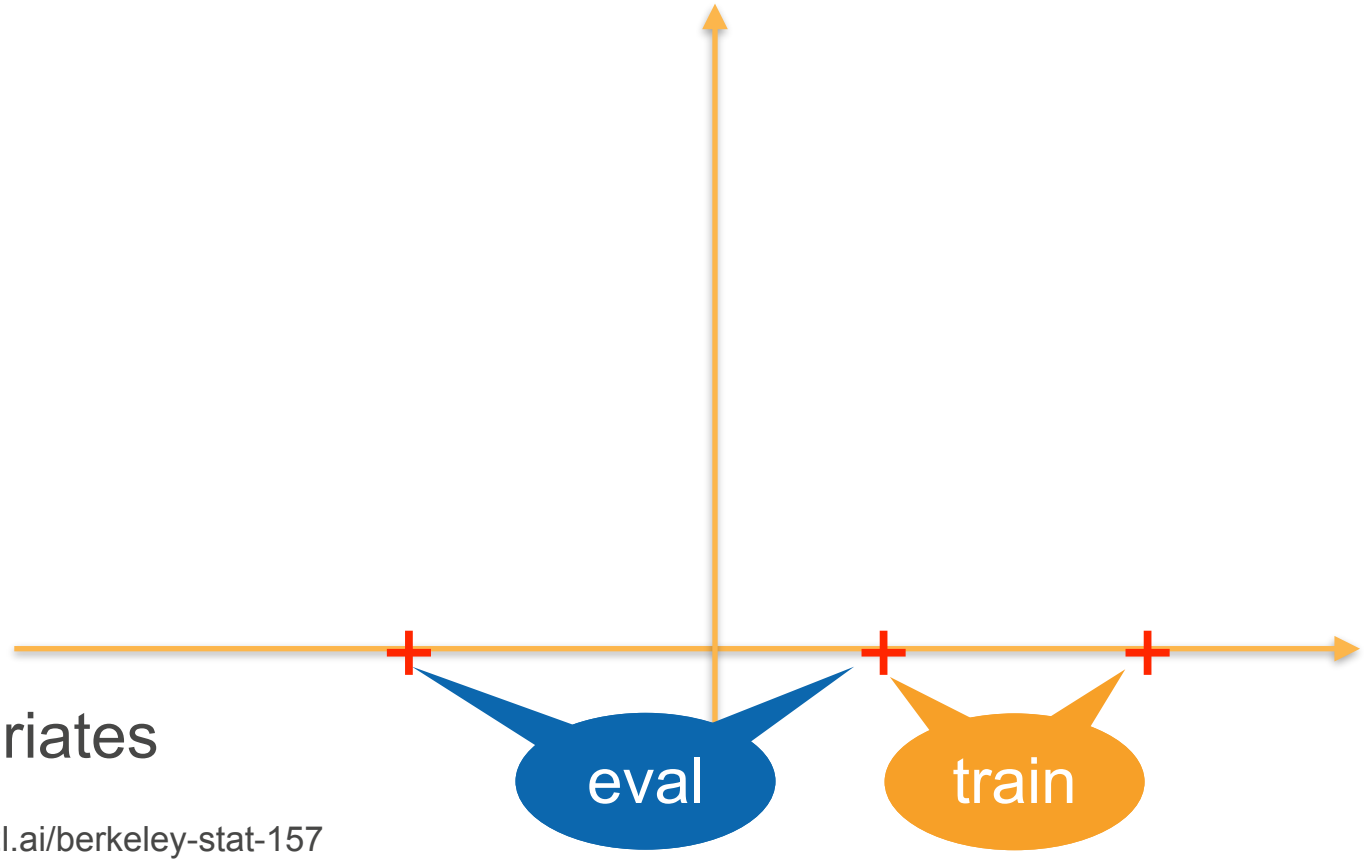
Simple regression problem



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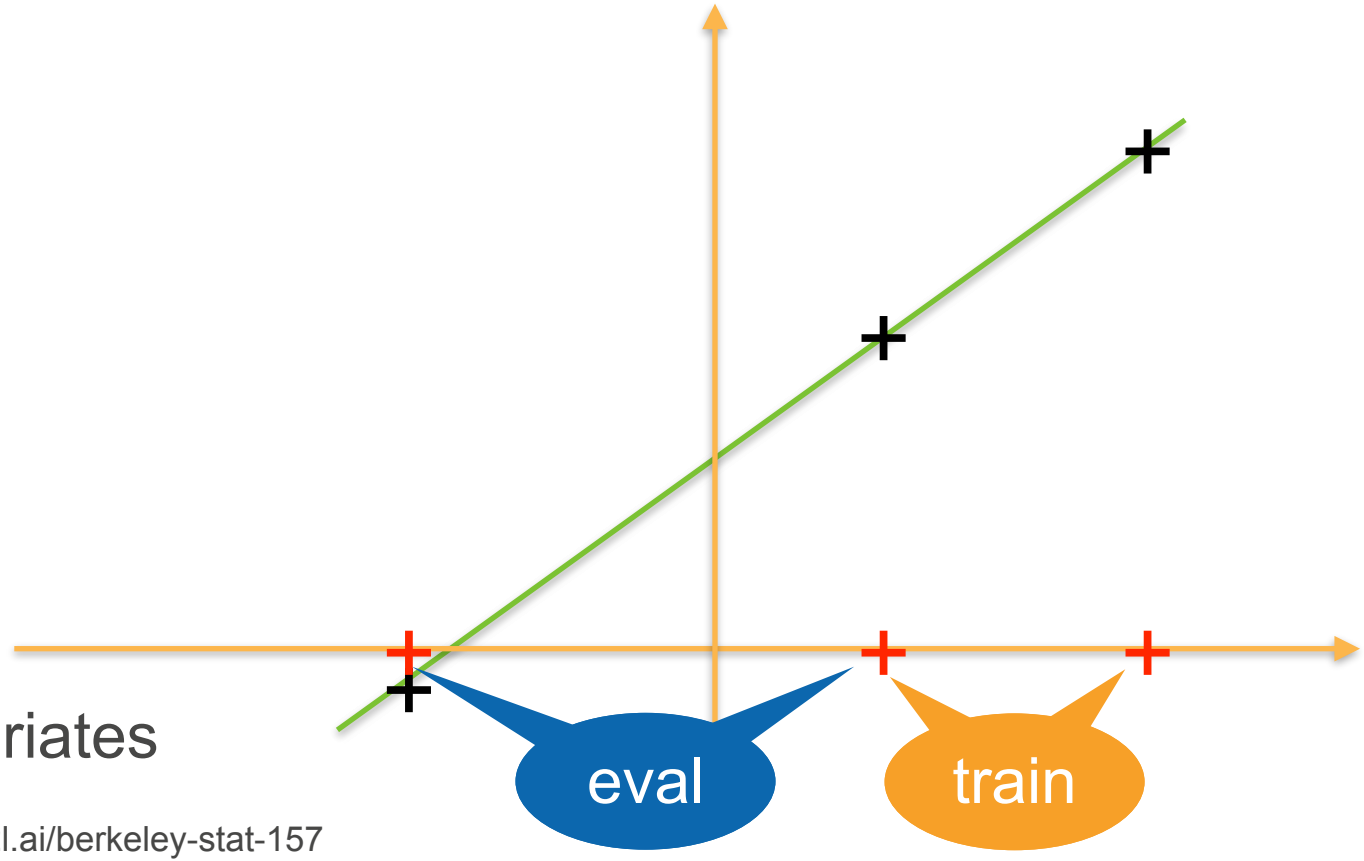
Simple regression problem



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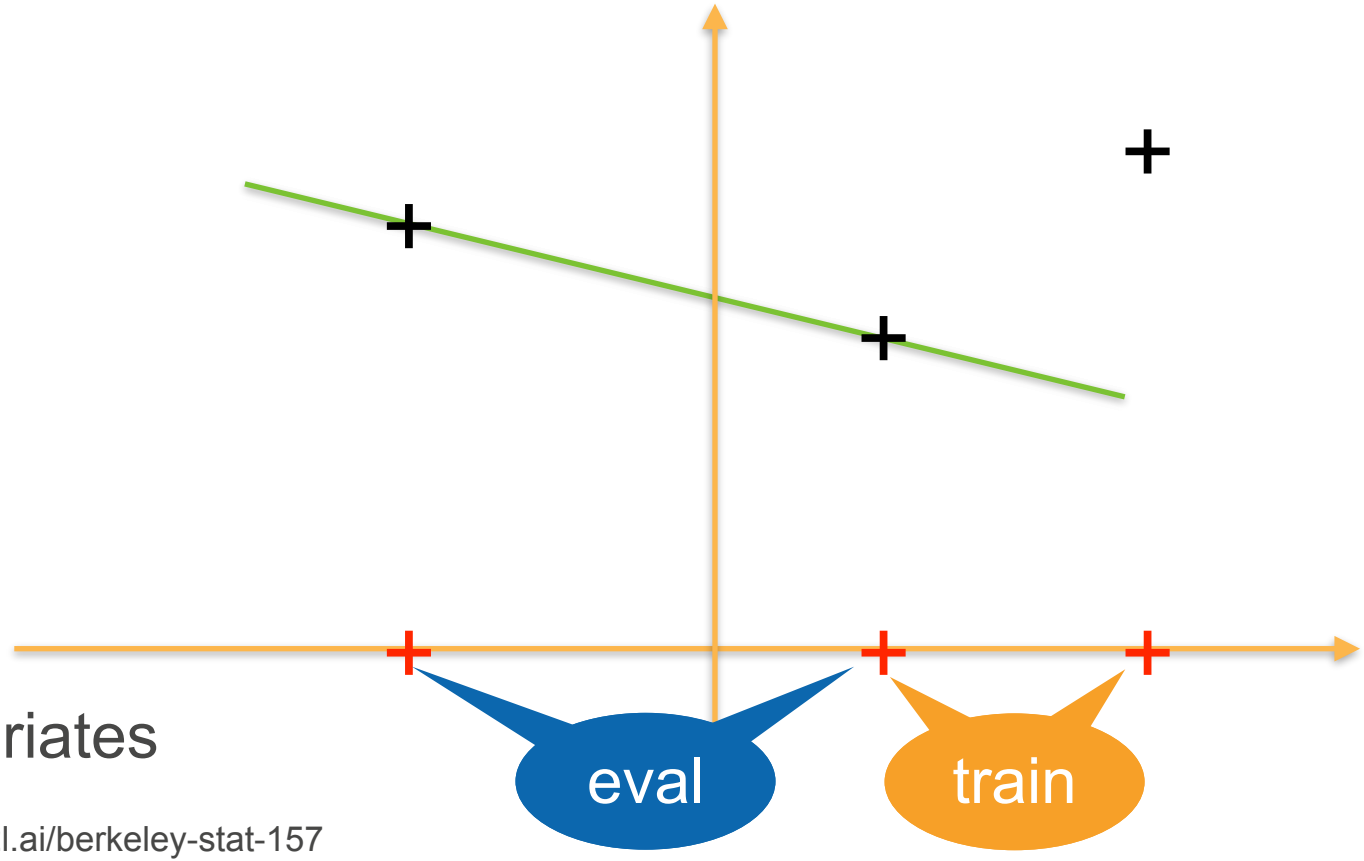
Simple regression problem



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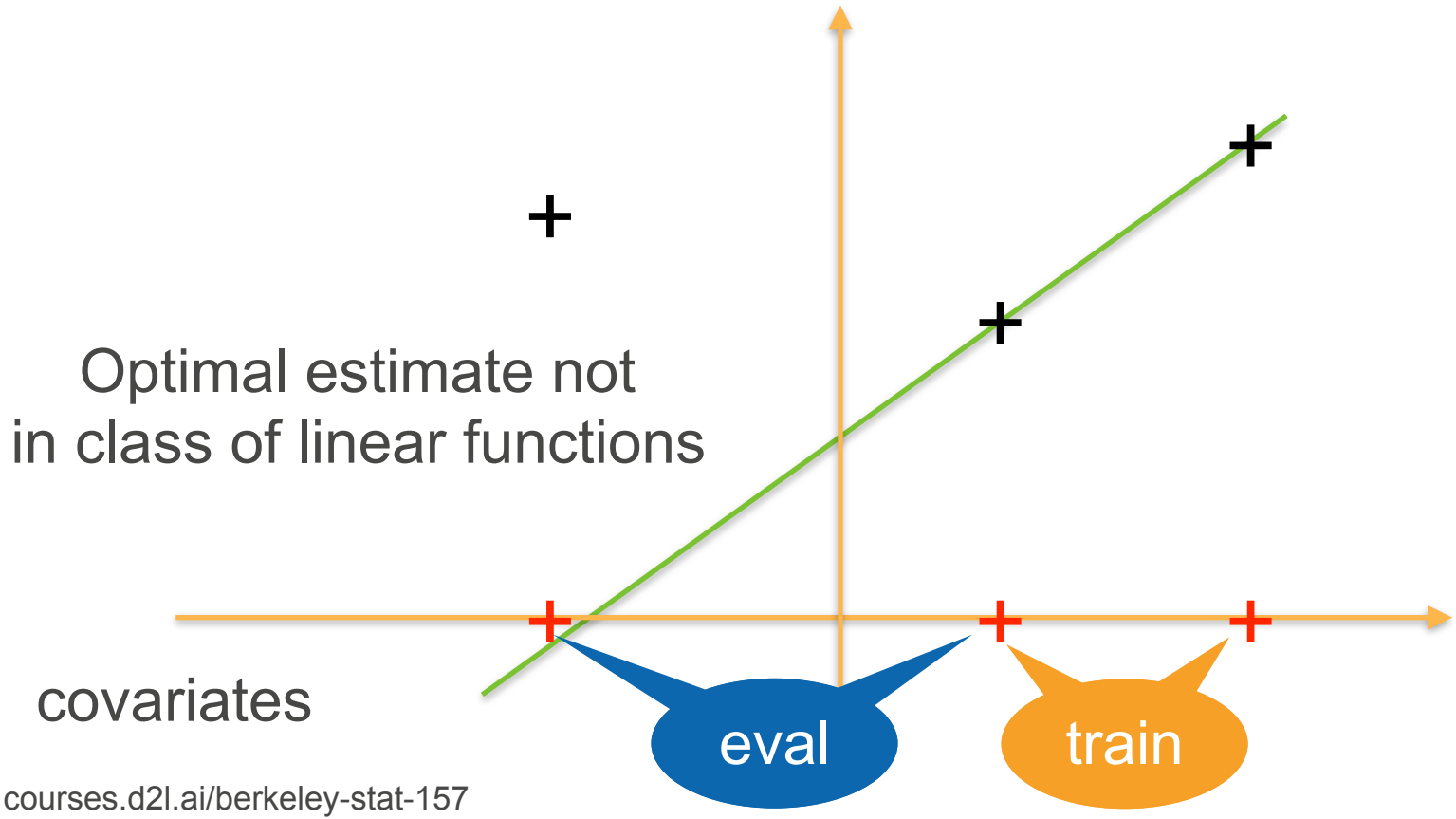
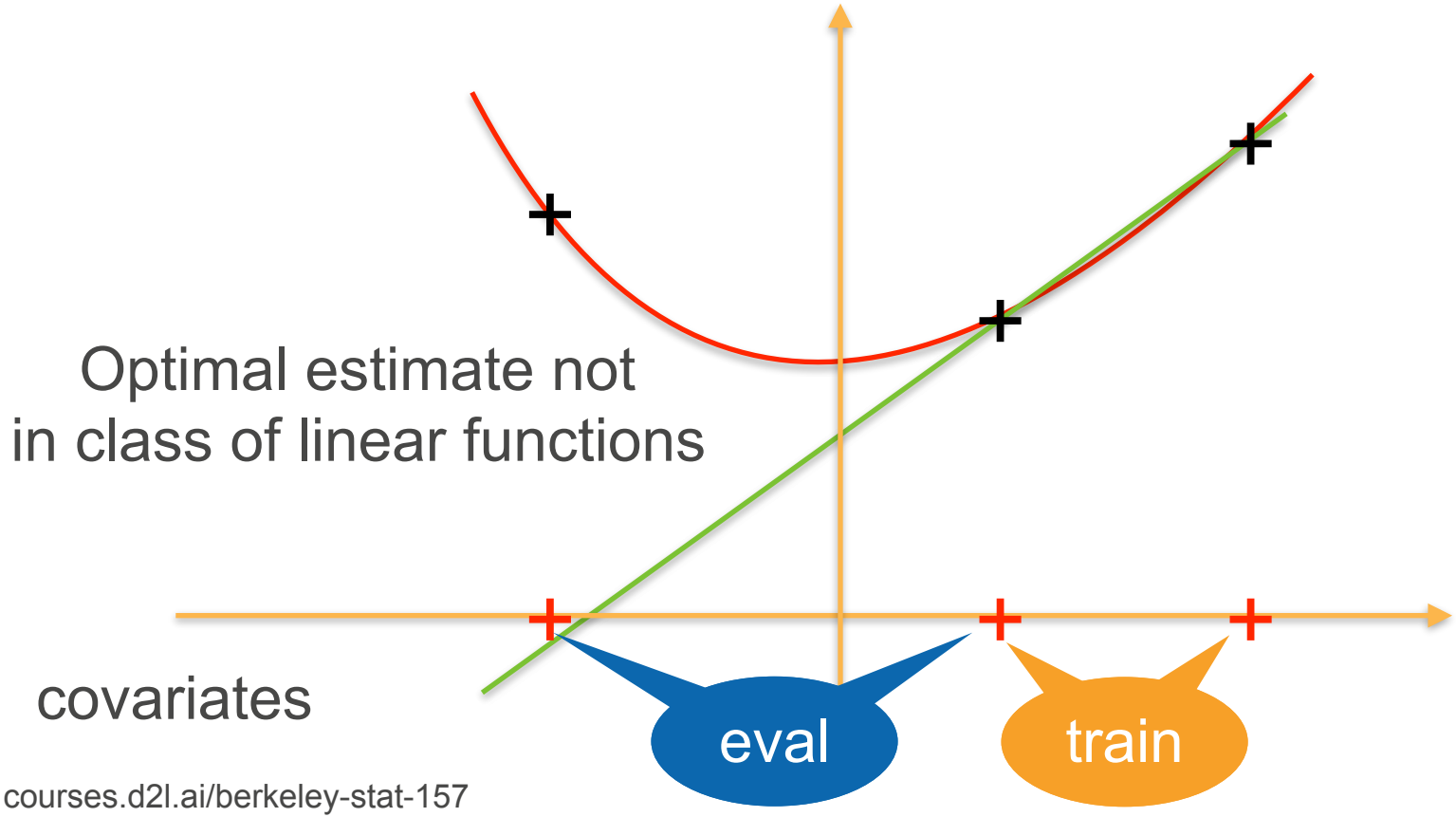
Simple regression problem



Simple regression problem



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

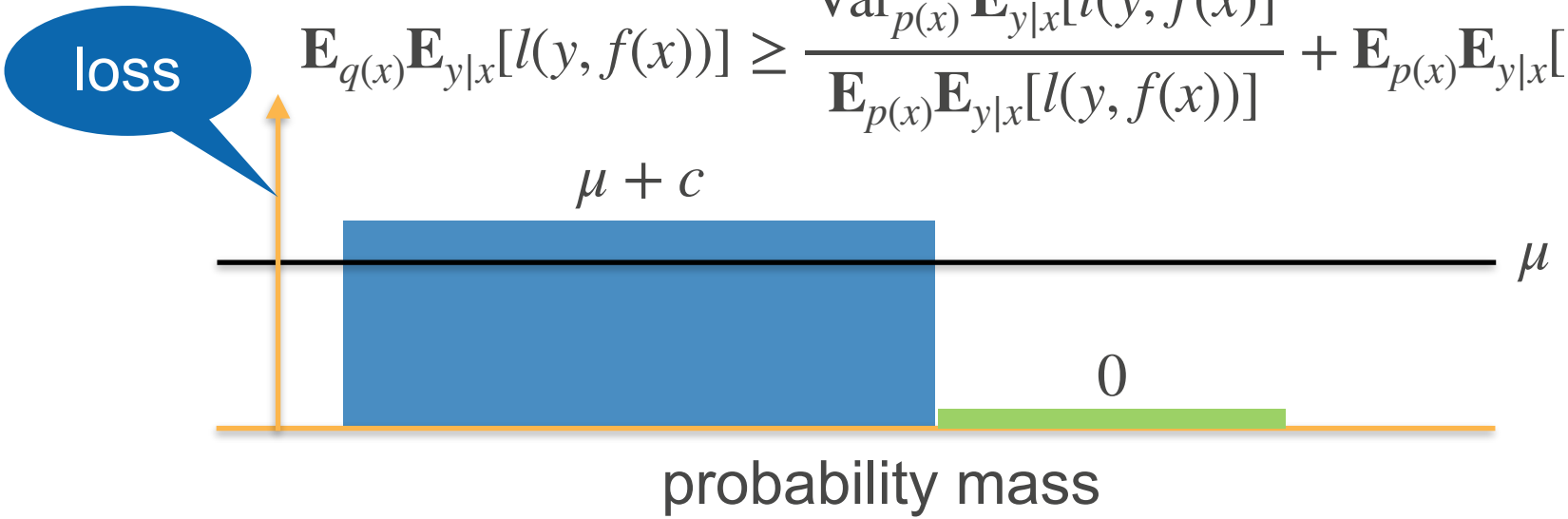
Train on IMDB

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.

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LOGISTIC
REGRESSION

Recall - Multiclass Classification

Calibrated Scale

- Output matches probabilities (nonnegative, sums to 1)

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

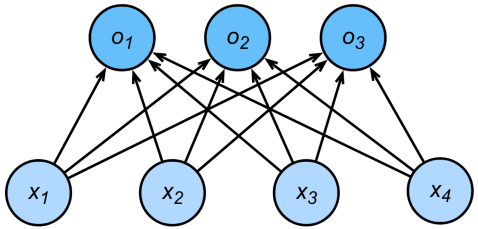
$$= \frac{\exp(o_y)}{\sum_i \exp(o_i)}$$

- 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 …



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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

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

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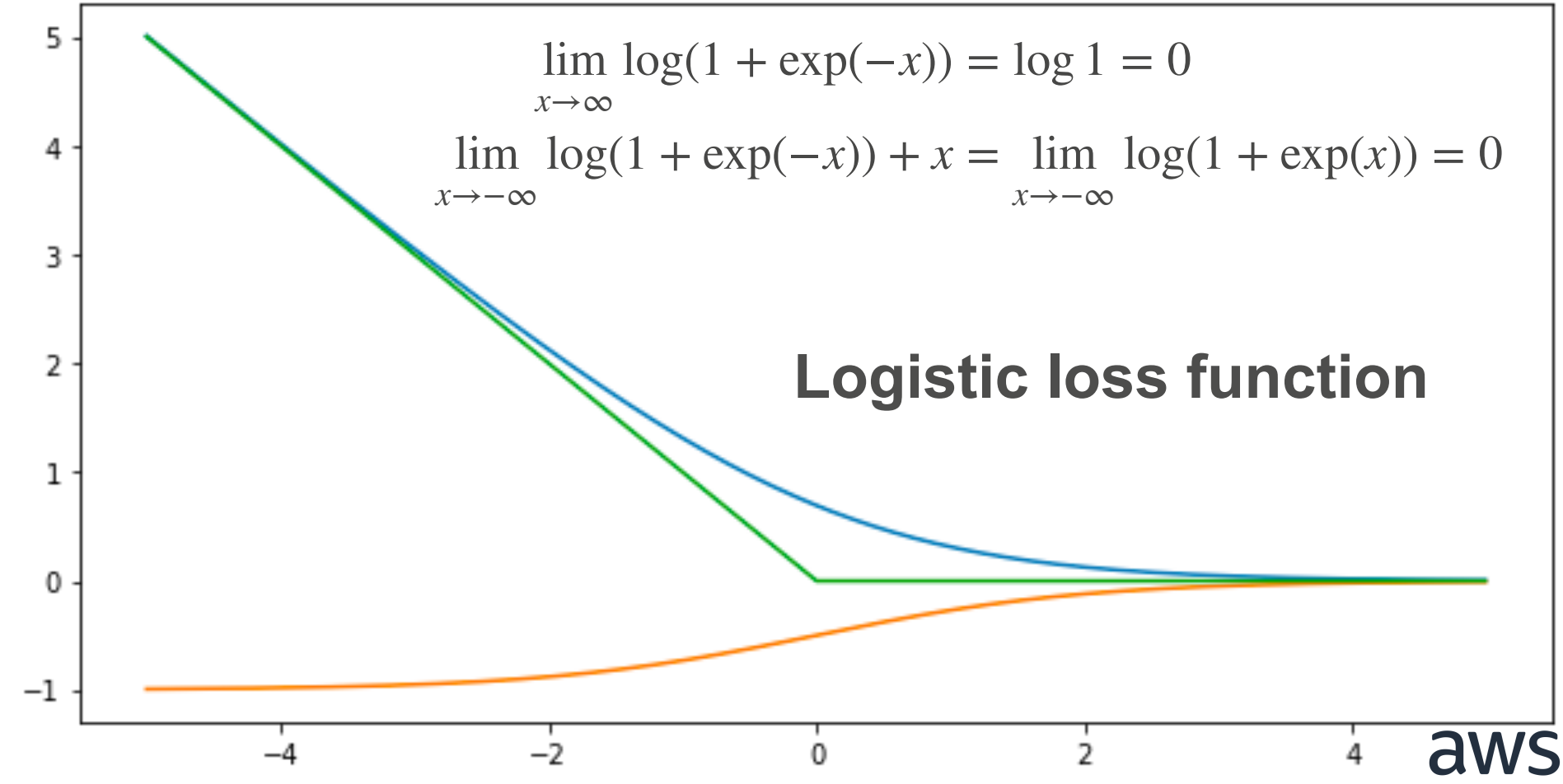

$\lim_{x \to \infty} \log(1 + \exp(-x)) = \log 1 = 0$
$\lim_{x \to -\infty} \log(1 + \exp(-x)) + x = \lim_{x \to -\infty} \log(1 + \exp(x)) = 0$
Logistic loss function
5
4
3
2
1
0
−1
−4
−2
0
2
4

Logistic Regression Summary

- **Data**

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

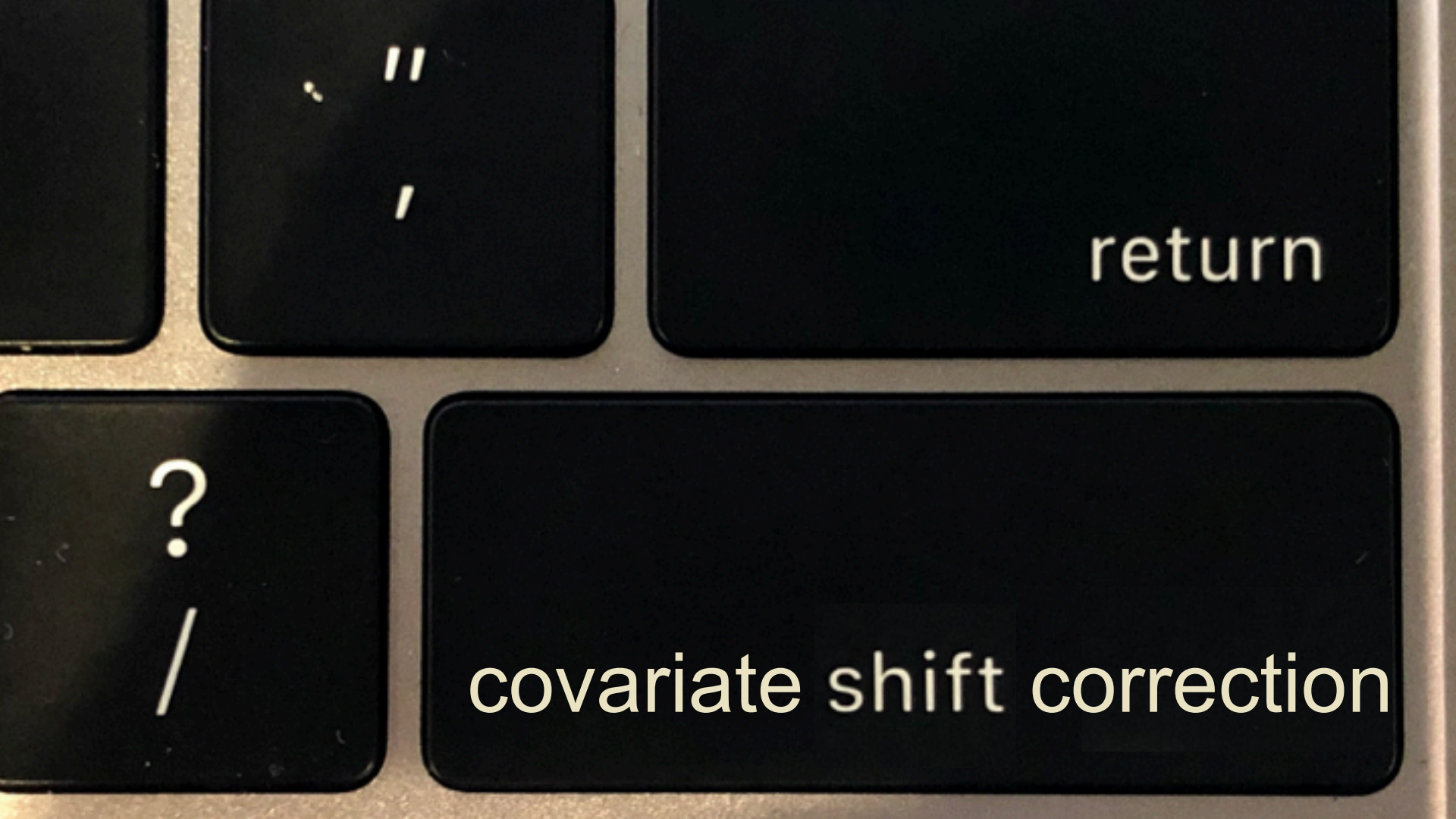
- **Objective**

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

- **Conditional Probability Estimate**

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

aws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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

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

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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

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

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

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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

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

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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)

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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)!

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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

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

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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

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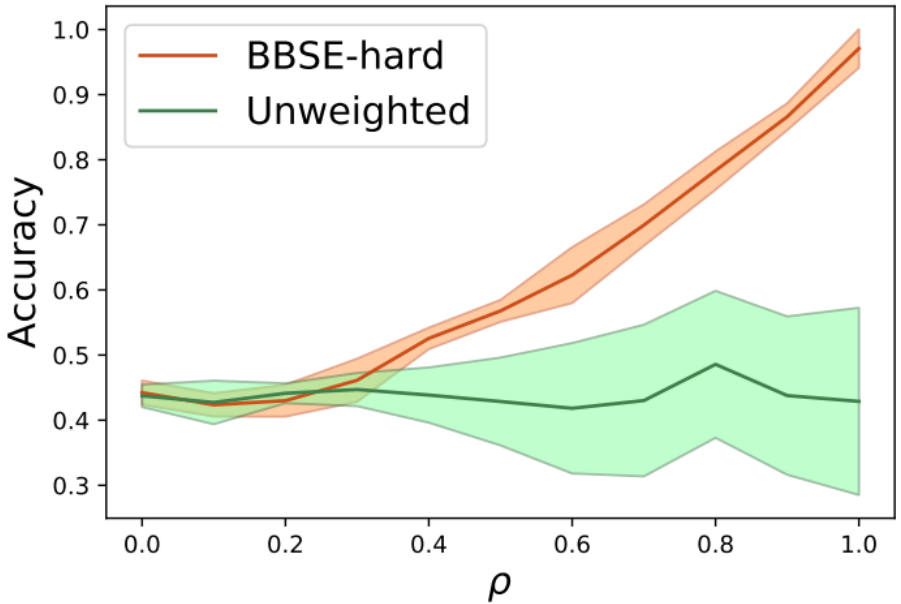
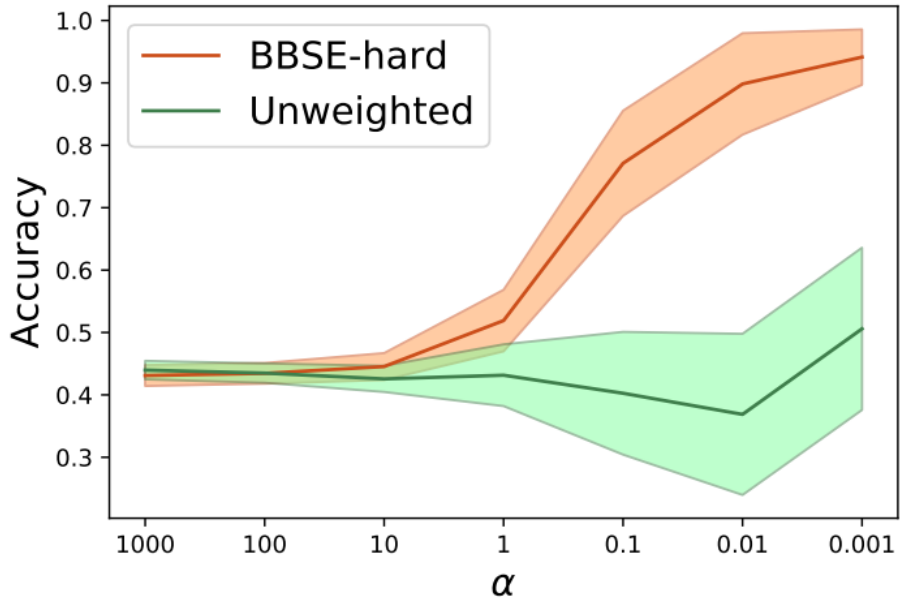
Black Box Shift Correction on CIFAR10



Tweaking one class probability



Dirichlet prior over shifts

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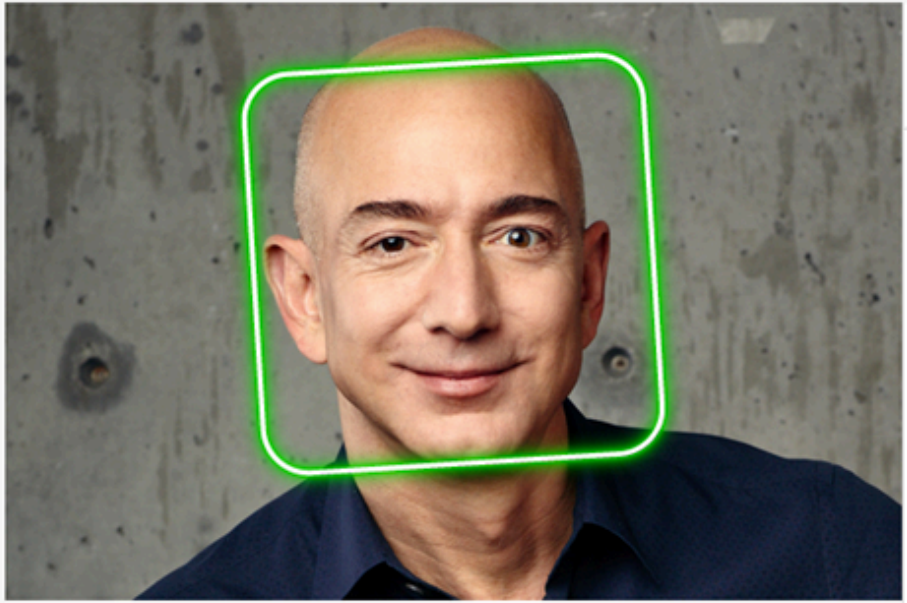
Adversarial data

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

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

Digital manipulation
to dodge recognition

In real life - via 3D
printed glasses

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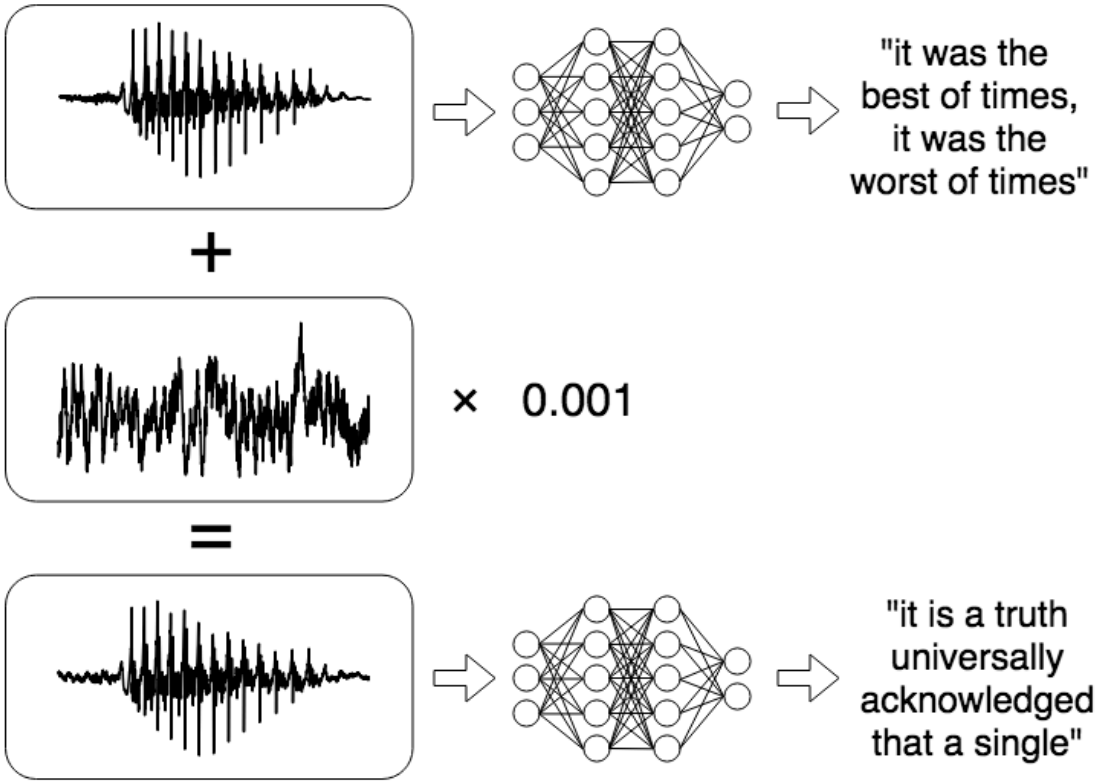
Adversarial Audio Generation (e.g. Carlini & Wagner, 2018)



- 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 …

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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

aws

‘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

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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, …’)

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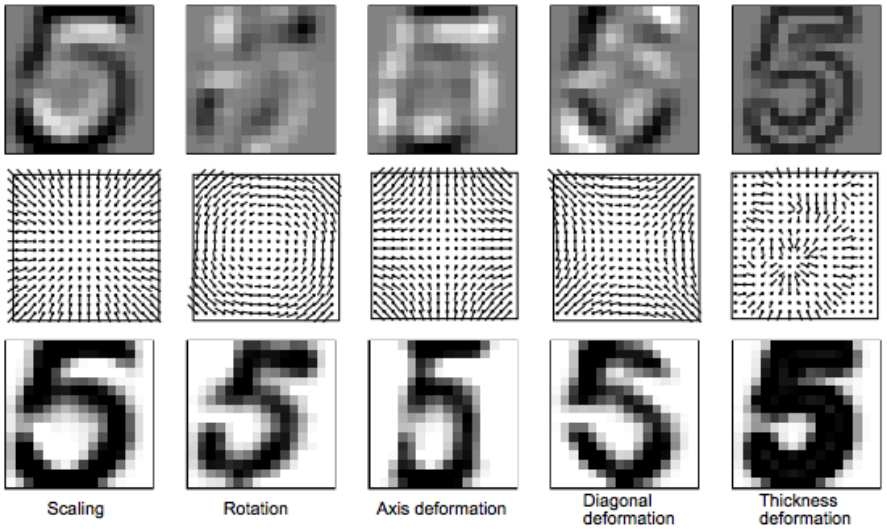
Invariances

- 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

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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

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Nonstationary Environments

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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

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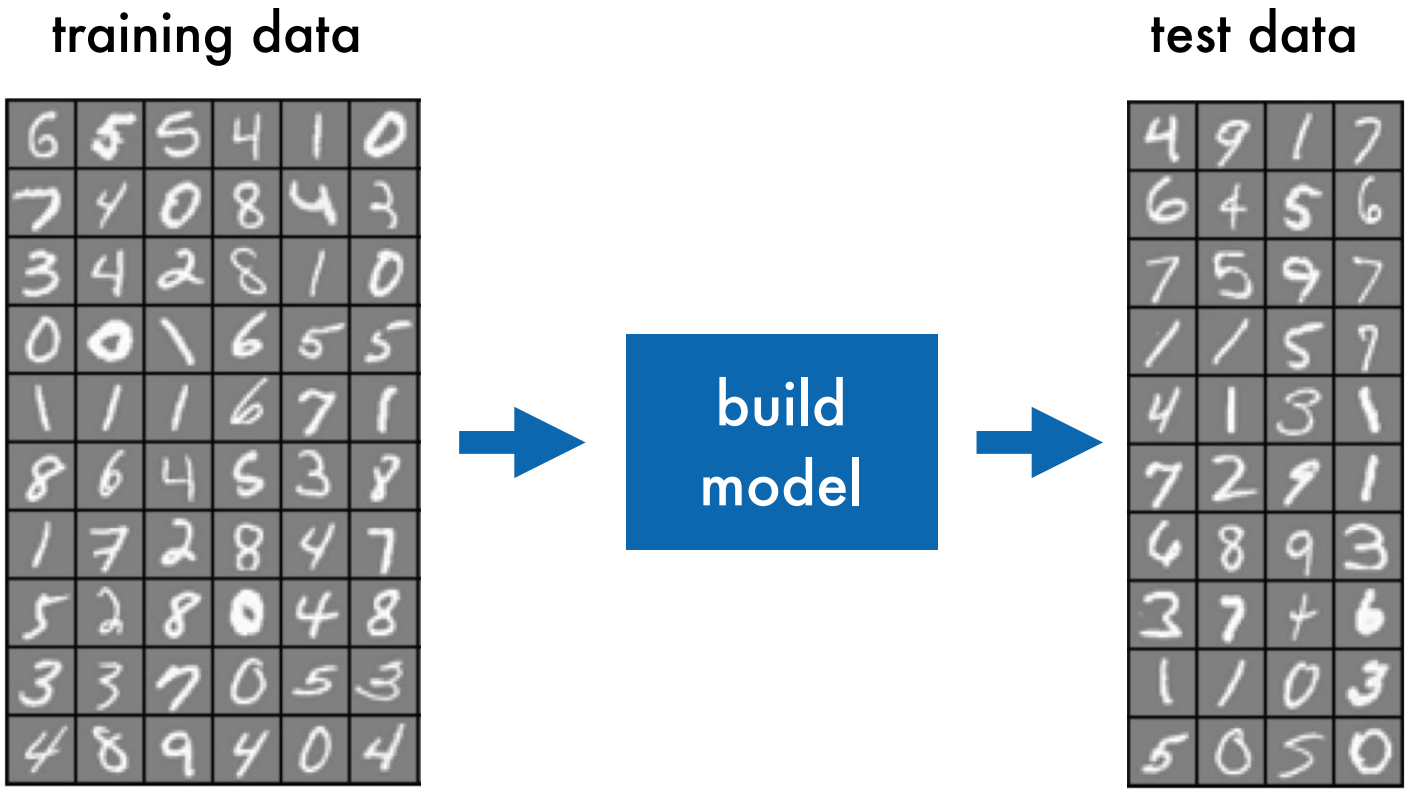
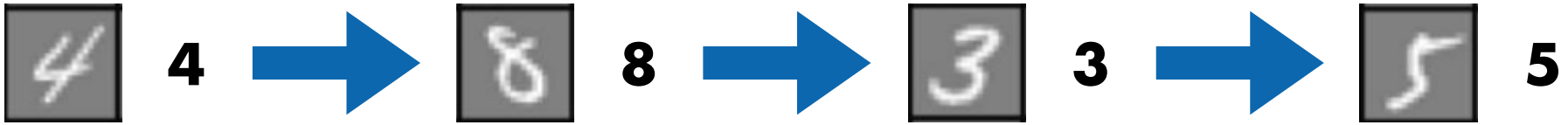
Batch



Online



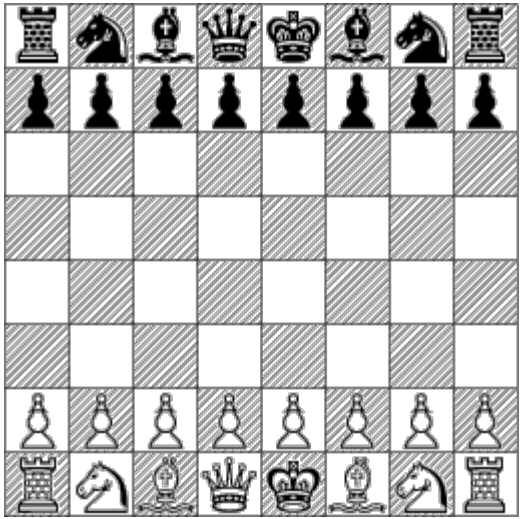
System improves as we see more data

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)

aws

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)

aws

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

Numerical Stability

Wikipedia

Gradients for Neural Networks

- Consider a network with *d* layers

$$\mathbf{h}^t = f_t(\mathbf{h}^{t-1}) \quad \text{and} \quad y = \ell \circ f_d \circ \ldots \circ f_1(\mathbf{x})$$

- Compute the gradient of the loss ℓ w.r.t. $\mathbf{W}_t$

$$\frac{\partial \ell}{\partial \mathbf{W}^t} = \frac{\partial \ell}{\partial \mathbf{h}^d} \underbrace{\frac{\partial \mathbf{h}^d}{\partial \mathbf{h}^{d-1}} \cdots \frac{\partial \mathbf{h}^{t+1}}{\partial \mathbf{h}^t}} \frac{\partial \mathbf{h}^t}{\partial \mathbf{W}^t}$$

Multiplication of *d-t* matrices

aws

Two Issues for Deep Neural Networks

$$\prod_{i=t}^{d-1} \frac{\partial \mathbf{h}^{i+1}}{\partial \mathbf{h}^{i}}$$

Gradient Exploding

$$1.5^{100} \approx 4 \times 10^{17}$$

Gradient Vanishing

$$0.8^{100} \approx 2 \times 10^{-10}$$

aws

Example: MLP

- Assume MLP (without bias for simplicity)

$$f_t(\mathbf{h}^{t-1}) = \sigma(\mathbf{W}^t\mathbf{h}^{t-1}) \qquad \sigma \text{ is the activation function}$$

$$\frac{\partial \mathbf{h}^t}{\partial \mathbf{h}^{t-1}} = \text{diag}\left(\sigma'(\mathbf{W}^t\mathbf{h}^{t-1})\right)(W^t)^T \qquad \sigma' \text{ is the gradient function of } \sigma$$

$$\prod_{i=t}^{d-1} \frac{\partial \mathbf{h}^{i+1}}{\partial \mathbf{h}^i} = \prod_{i=t}^{d-1} \text{diag}\left(\sigma'(\mathbf{W}^i\mathbf{h}^{i-1})\right)(W^i)^T$$

aws

Gradient Exploding

- Use ReLU as the activation function

$$\sigma(x) = \max(0,x) \quad \text{and} \quad \sigma'(x) = \begin{cases} 1 & \text{if } x > 0 \\ 0 & \text{otherwise} \end{cases}$$

- Elements of $\prod_{i=t}^{d-1} \frac{\partial \mathbf{h}^{i+1}}{\partial \mathbf{h}^i} = \prod_{i=t}^{d-1} \text{diag}\left(\sigma'(\mathbf{W}^i \mathbf{h}^{i-1})\right)(W^i)^T$ may from $\prod_{i=t}^{d-1} (W^i)^T$
  - Leads to large values when *d-t* is large

$$1.5^{100} \approx 4 \times 10^{17}$$

aws

Issues with Gradient Exploding

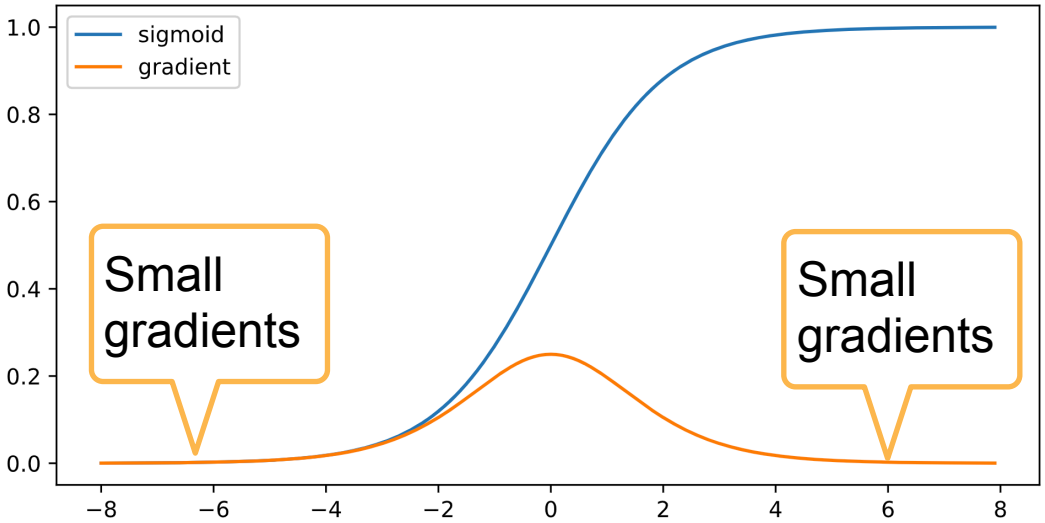
- Value out of range: infinity value
  - Severe for using 16-bit floating points
    - Range: 6e-5 - 6e4
- Sensitive to learning rate (LR)
  - Not small enough LR -> large weights -> larger gradients
  - Too small LR -> No progress
  - May need to change LR dramatically during training

aws

Gradient Vanishing

- Use sigmoid as the activation function

$$\sigma(x) = \frac{1}{1 + e^{-x}} \qquad \sigma'(x) = \sigma(x)(1 - \sigma(x))$$



Gradient Exploding

- Use sigmoid as the activation function

$$\sigma(x) = \frac{1}{1 + e^{-x}} \qquad \sigma'(x) = \sigma(x)(1 - \sigma(x))$$

- Elements $\prod_{i=t}^{d-1} \frac{\partial \mathbf{h}^{i+1}}{\partial \mathbf{h}^{i}} = \prod_{i=t}^{d-1} \text{diag}\left(\sigma'(\mathbf{W}^i \mathbf{h}^{i-1})\right)(W^i)^T$ are products of *d-t* small values

$$0.8^{100} \approx 2 \times 10^{-10}$$

aws

Issues with Gradient Vanishing

- Gradients with value 0
  - Severe with 16-bit floating points
- No progress in training
  - No matter how to choose learning rate
- Severe with bottom layers
  - Only top layers are well trained
  - No benefit to make networks deeper

aws

Stabilize Training

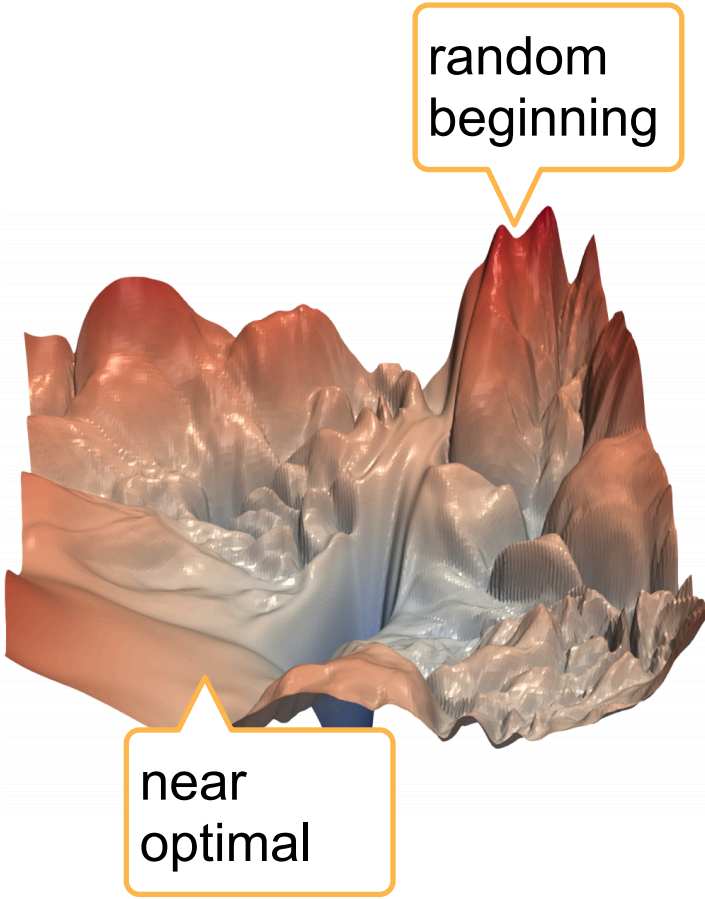
Stabilize Training

- Goal: make sure gradient values are in a proper range
  - E.g. in [1e-6, 1e3]
- Multiplication -> plus
  - ResNet, LSTM
- Normalize
  - Batch Normalization, Gradient clipping
- Proper weight initialization and activation functions

aws

Weight Initialization

- Initialize weights with random values in a proper range
- The beginning of training easily suffers to numerical instability
  - The surface far away from an optimal can be complex
  - Near optimal may be flatter
- Initializing according to $\mathcal{N}(0, 0.01)$ works well for small networks, but not guarantee for deep neural networks



Constant Variance for each Layer

- Treat both layer outputs and gradients are random variables
- Make the mean and variance for each layer's output are same, similar for gradients

Forward

$$\mathbb{E}[h_i^t] = 0$$

$$\mathrm{Var}[h_i^t] = a$$

Backward

$$\mathbb{E}\left[\frac{\partial \ell}{\partial h_i^t}\right] = 0 \quad \mathrm{Var}\left[\frac{\partial \ell}{\partial h_i^t}\right] = b \qquad \forall i, t$$

a and *b* are constants

aws

Example: MLP

- Assumptions
  - i.i.d $w_{i,j}^t$, $\mathbb{E}[w_{i,j}^t] = 0, \mathrm{Var}[w_{i,j}^t] = \gamma_t$
  - h_i^{t-1} is independent to $w_{i,j}^t$
  - identity activation: $\mathbf{h}^t = \mathbf{W}^t \mathbf{h}^{t-1}$ with $\mathbf{W}^t \in \mathbb{R}^{n_t \times n_{t-1}}$

$$\mathbb{E}[h_i^t] = \mathbb{E}\left[\sum_j w_{i,j}^t h_j^{t-1}\right] = \sum_j \mathbb{E}[w_{i,j}^t]\mathbb{E}[h_j^{t-1}] = 0$$

aws

Forward Variance

$$\mathrm{Var}[h_i^t] = \mathbb{E}[(h_i^t)^2] - \mathbb{E}[h_i^t]^2 = \mathbb{E}\left[\left(\sum_j w_{i,j}^t h_j^{t-1}\right)^2\right]$$

$$= \mathbb{E}\left[\sum_j \left(w_{i,j}^t\right)^2 \left(h_j^{t-1}\right)^2 + \sum_{j \neq k} w_{i,j}^t w_{i,k}^t h_j^{t-1} h_k^{t-1}\right] \quad \Rightarrow \quad n_{t-1}\gamma_t = 1$$

$$= \sum_j \mathbb{E}\left[\left(w_{i,j}^t\right)^2\right] \mathbb{E}\left[\left(h_j^{t-1}\right)^2\right]$$

$$= \sum_j \mathrm{Var}[w_{i,j}^t]\mathrm{Var}[h_j^{t-1}] = n_{t-1}\gamma_t \mathrm{Var}[h_j^{t-1}]$$

aws

Backward Mean and Variance

- Apply forward analysis as well

$$\frac{\partial \ell}{\partial \mathbf{h}^{t-1}} = \frac{\partial \ell}{\partial \mathbf{h}^{t}} \mathbf{W}^{t} \quad \text{leads to} \quad \left(\frac{\partial \ell}{\partial \mathbf{h}^{t-1}} \right)^{T} = (W^{t})^{T} \left(\frac{\partial \ell}{\partial \mathbf{h}^{t}} \right)^{T}$$

$$\mathbb{E}\left[\frac{\partial \ell}{\partial h_i^{t-1}} \right] = 0$$

$$\mathrm{Var}\left[\frac{\partial \ell}{\partial h_i^{t-1}} \right] = n_t \gamma_t \mathrm{Var}\left[\frac{\partial \ell}{\partial h_j^{t}} \right] \quad \Rightarrow \quad n_t \gamma_t = 1$$

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Xavier Initialization

- Conflict goal to satisfies both $n_{t-1}\gamma_t = 1$ and $n_t\gamma_t = 1$
- Xavier $\gamma_t(n_{t-1} + n_t)/2 = 1 \quad \rightarrow \quad \gamma_t = 2/(n_{t-1} + n_t)$
  - Normal distribution $\mathcal{N}\left(0, \sqrt{2/(n_{t-1} + n_t)}\right)$
  - Uniform distribution $\mathcal{U}\left(-\sqrt{6/(n_{t-1} + n_t)}, \sqrt{6/(n_{t-1} + n_t)}\right)$
    - Variance of $\mathcal{U}[-a, a]$ is $a^2/3$
- Adaptive to weight shape, especially when n_t varies

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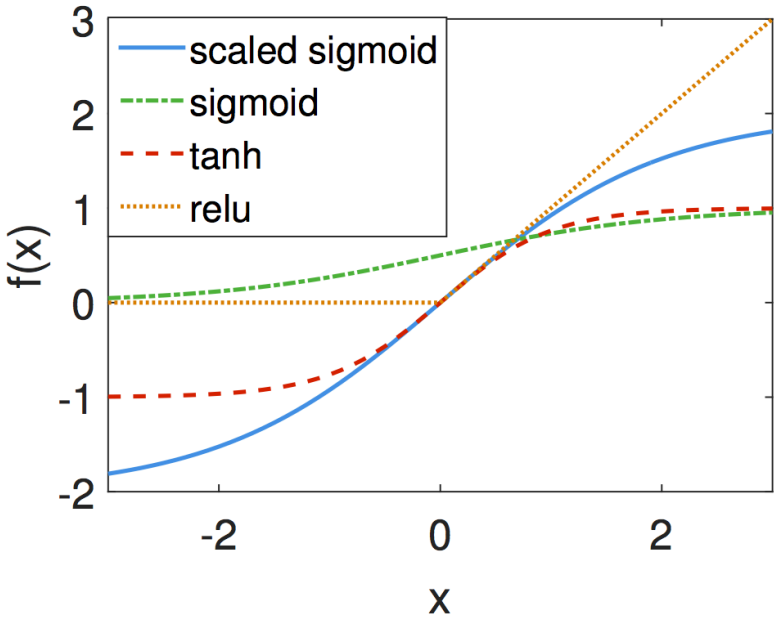
Activation



A Simple Linear Activation Function

- Assume $\sigma(x) = \alpha x + \beta$

$$\mathbf{h}' = \mathbf{W}^t \mathbf{h}^{t-1} \quad \text{and} \quad \mathbf{h}^t = \sigma(\mathbf{h}')$$

$$\mathbb{E}[h_i^t] = \mathbb{E}\left[\alpha h_i' + \beta\right] = \beta \quad \Rightarrow \quad \beta = 0$$

$$\begin{aligned}
\mathrm{Var}[h_i^t] &= \mathbb{E}[(h_i^t)^2] - \mathbb{E}[h_i^t]^2 \\
&= \mathbb{E}[(\alpha h_i' + \beta)^2] - \beta^2 \quad \Rightarrow \quad \alpha = 1 \\
&= \mathbb{E}[\alpha^2 (h_i')^2 + 2\alpha\beta h_i' + \beta^2] - \beta^2 \\
&= \alpha^2 \mathrm{Var}[h_i']
\end{aligned}$$

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Backward

- Assume $\sigma(x) = \alpha x + \beta$

$$\frac{\partial \ell}{\partial \mathbf{h}'} = \frac{\partial \ell}{\partial \mathbf{h}^t}(W^t)^T \quad \text{and} \quad \frac{\partial \ell}{\partial \mathbf{h}^{t-1}} = \alpha \frac{\partial \ell}{\partial \mathbf{h}'}$$

$$\mathbb{E}\left[\frac{\partial \ell}{\partial h_i^{t-1}}\right] = 0 \quad \Rightarrow \quad \beta = 0$$

$$\mathrm{Var}\left[\frac{\partial \ell}{\partial h_i^{t-1}}\right] = \alpha^2 \mathrm{Var}\left[\frac{\partial \ell}{\partial h_j'}\right] \quad \Rightarrow \quad \alpha = 1$$

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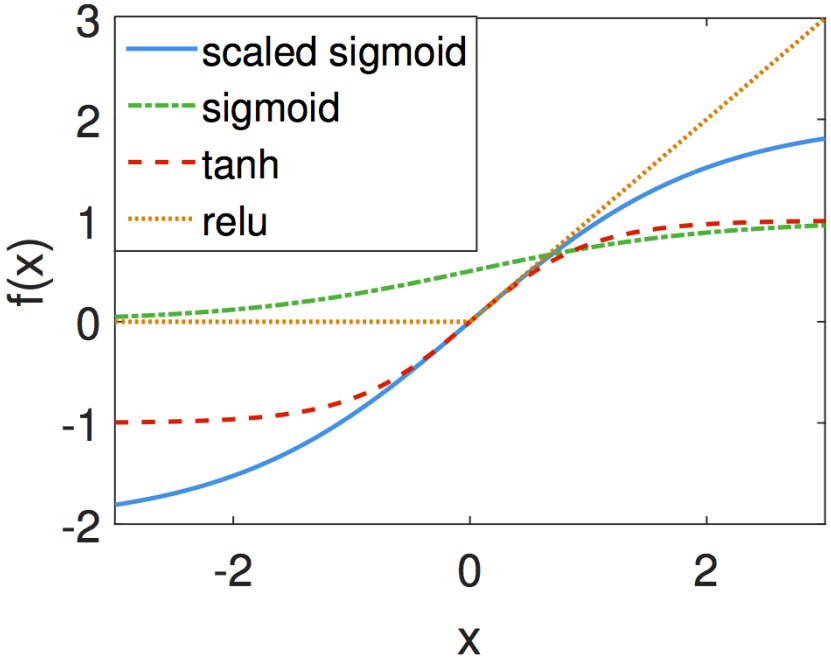
Revise Activation Functions

- By the Taylor expansions

$$\text{sigmoid}(x) = \frac{1}{2} + \frac{x}{4} - \frac{x^3}{48} + O(x^5)$$

$$\tanh(x) = 0 + x - \frac{x^3}{3} + O(x^5)$$

$$\text{relu}(x) = 0 + x \quad \text{for } x \geq 0$$



- "Correct" sigmoid by

$$4 \times \text{sigmoid}(x) - 2$$

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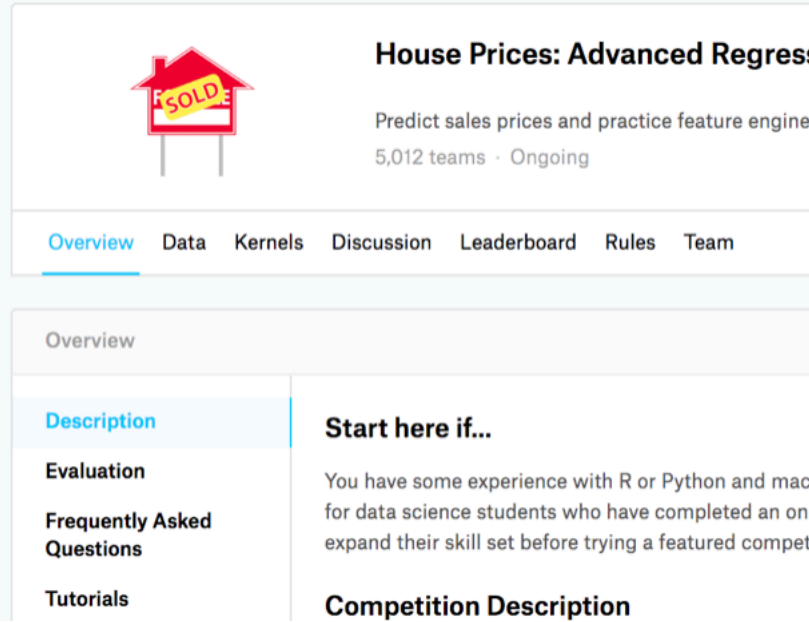
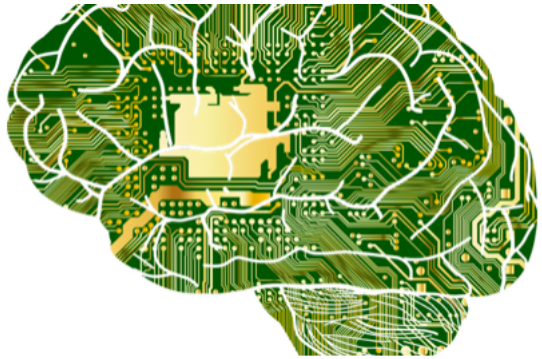
Predicting House Prices on Kaggle



Hardware for Deep Learning



(articleshub360.com)

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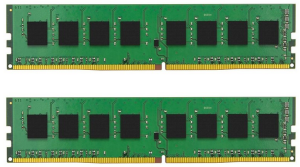
Your GPU Computer

Intel i7
0.15 TFLOPS



DDR4
32 GB

Nvidia Titan X
12 TFLOPS
16 GB

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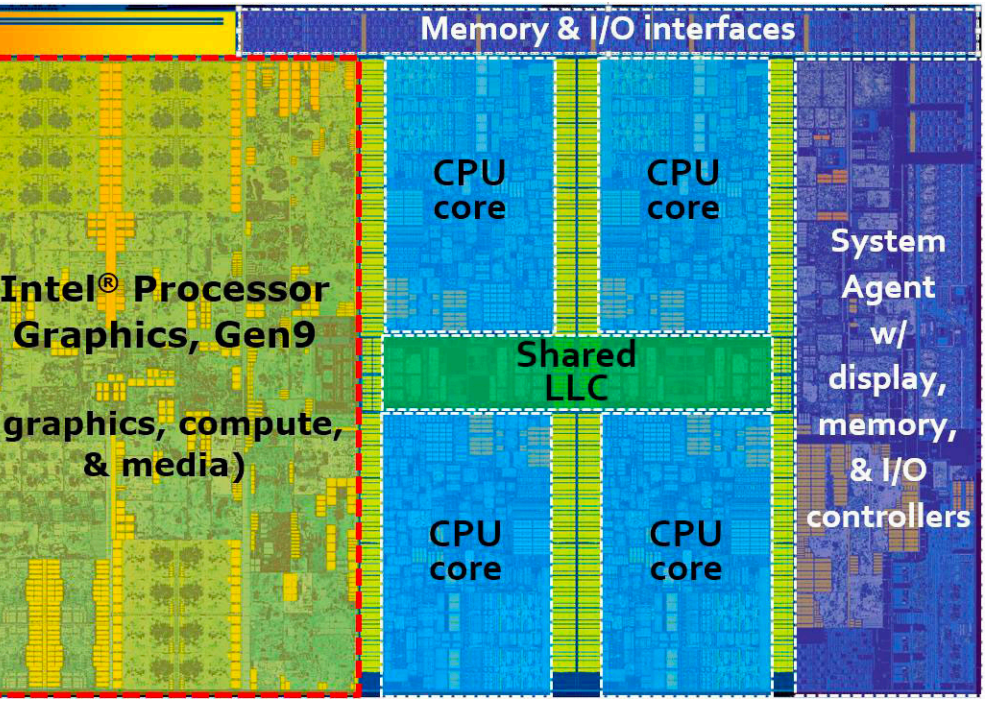
Intel i7-6700K



- 4 Physical cores
- Per core
  - 64KB L1 cache
  - 256KB L2 cache
- Shared 8MB L3 cache
- 30 GB/s to main memory

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Improve CPU Utilization I

- Before computing *a* + *b*, need to prepare data first
  - Main memory -> L3 -> L2 -> L1 -> registers
    - L1 cache reference time: 0.5 ns
    - L2 cache reference time 7 ns (14 x L1)
    - Main memory reference time 100ns (200 x L1)
- Improve temporal and spatial memory locality
  - Temporal: reuse data so we keep them on cache
  - Spatial: read data sequential so we can pre-fetch data

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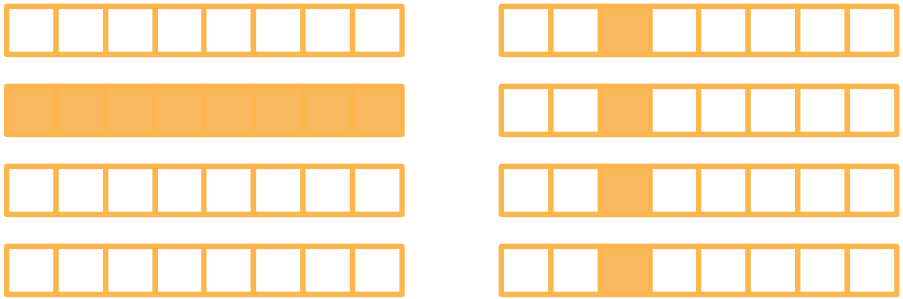
Case Study

- For a matrix stored in raw-major, accessing a column is slower than accessing a row
  - CPU reads 64 bytes (cache line) each time
  - CPU “smartly” reads the next cache line ahead when it’s needed



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Improve CPU Utilization II

- Server CPUs may have dozens of cores
  - EC2 P3.16xlarge: 2 Intel Xeon CPUs, 32 physical cores in total
- Parallelization to use all cores
  - Hyper-threading may not help because of shared registers

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Case Study

- Left is slower than right (Python)

```
for i in range(len(a)):
    c[i] = a[i] + b[i]
```

```
c = a + b
```

  - Left issues *n* calls, each invoking has certain overhead (e.g. several microsecond)
  - Right is easier to be parallelized by a C++ operator

```
#pragma omp for
for (i=0; i<a.size(); i++) {
    c[i] = a[i] + b[i]
}
```


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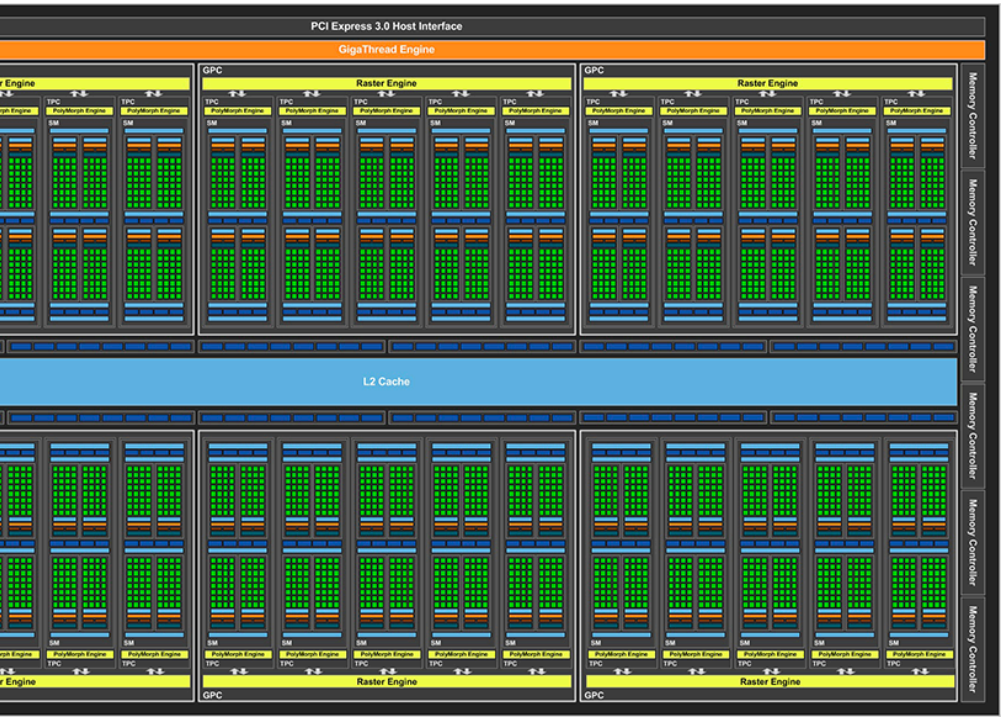
Nvidia Titan X (Pascal)



- 2584 cores, each core
  - Multiple arithmetic units
- 3MB L2 cache
- 480 GB/s memory bandwidth

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Improve GPU Utilization

- Parallelization
  - Uses thousands of threads
- Memory locality
  - Simple cache architecture and small cache size
- Simple control flows
  - Very limited support
  - Large synchronization

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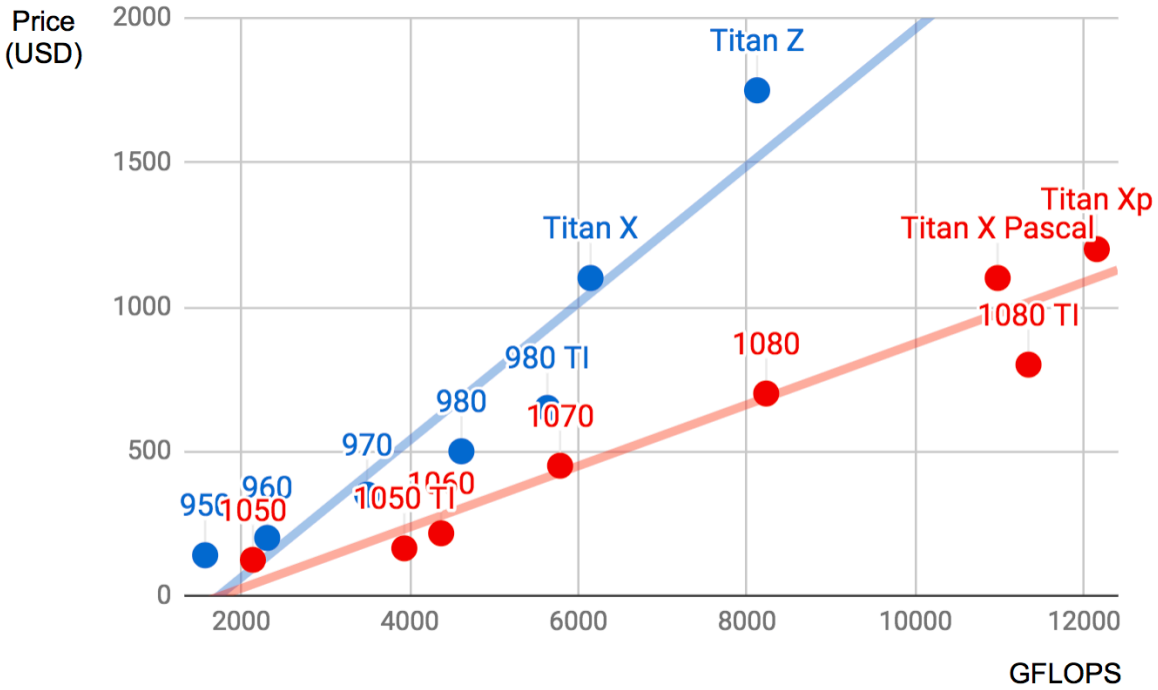
Buy GPUs



- Each series improve the previous one
  - Buy new models
- Price is linear to power in a series

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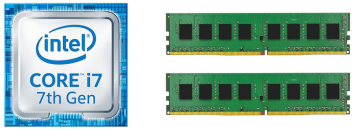
CPU vs GPU



# Cores	6 / 64	2K / 4K
TFLOPS	0.2 / 1	10 / 100
Memory size	32 GB / 1 TB	16 GB / 32 GB
Memory bandwidth	30 GB/s / 100 GB/s	400 GB/s / 1 TB/s
Control flow	Strong	Weak

Typical / High End

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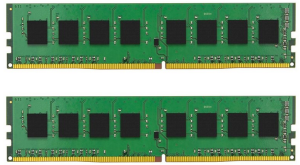
CPU/GPU Bandwidth

30 GB/s



PCIe 3.0 16x: 16 GB/s

480 GB/s

- Do not copy data between GPU and CPU frequently
  - Limited PCIe bandwidth
  - Synchronization overhead

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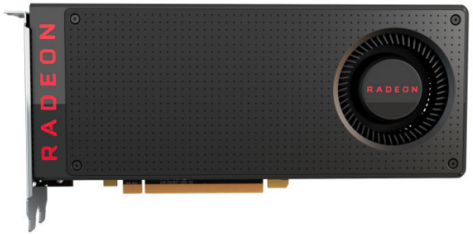
More CPUs and GPUs

- CPU
  - Desktop/Server: AMD
  - Edge: ARM
- GPU
  - Desktop/Server GPU: AMD, Intel
  - Edge: ARM, Qualcomm



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Programming on CPU/GPU

- CPU: C++ or any other high-performance language
  - Mature compilers with performance guaranteed
- GPU
  - CUDA for Nvidia
    - Rich features, mature complier and driver
  - OpenCL for others
    - Quality varies for chip vendors

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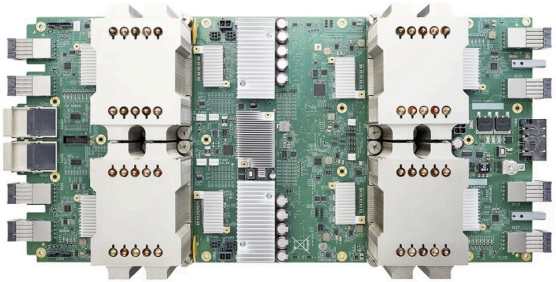
More Promising Hardware



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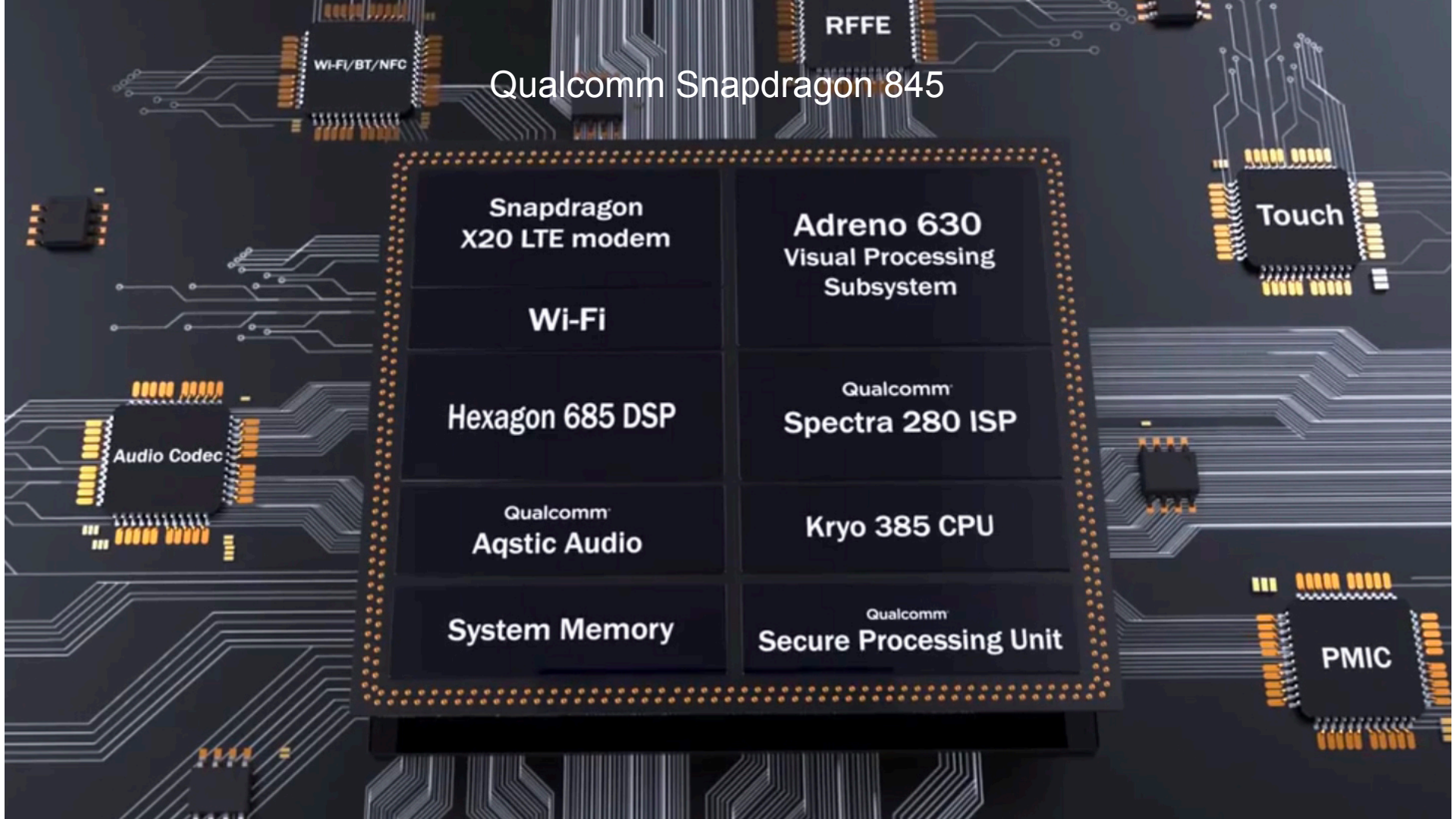
Qualcomm Snapdragon 845
Wi-Fi/BT/NFC
RFFE
Touch
Audio Codec
PMIC
Snapdragon
X20 LTE modem
Wi-Fi
Adreno 630
Visual Processing
Subsystem
Hexagon 685 DSP
Qualcomm
Spectra 280 ISP
Qualcomm
Aqstic Audio
Kryo 385 CPU
System Memory
Qualcomm
Secure Processing Unit

Digital Signal Processor

- Designed for digital processing algorithms
  - Dot product, Convolution, FFT
- Low power and high performance
  - 5x faster than mobile GPUs, uses less power
- VLIW: Very long instruction word
  - Hundreds multiply-accumulates in a single instruction
- Hard to program and debug
- Compiler toolchain quality varies from chip vendors

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Field-Programmable Gate Array (FPGA)

- Contains a large number of programmable logic blocks and reconfigurable interconnects
- Can be configured to perform complex functions
  - Common languages: VHDL and Verilog
- Often has high efficiency than general purpose hardware
- Toolchain qualities vary
- Each “compilation” may take several hours

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AI ASIC

- Hot topic in deep learning
  - Every major company is building their chips (Intel, Qualcomm, Google, Amazon, Facebook, …)
- Google TPU is a landmark chip
  - Matches high-end Nvidia GPU's performance, but 10x-100x cheaper
  - Widely deployed in Google
  - The core is a systolic array

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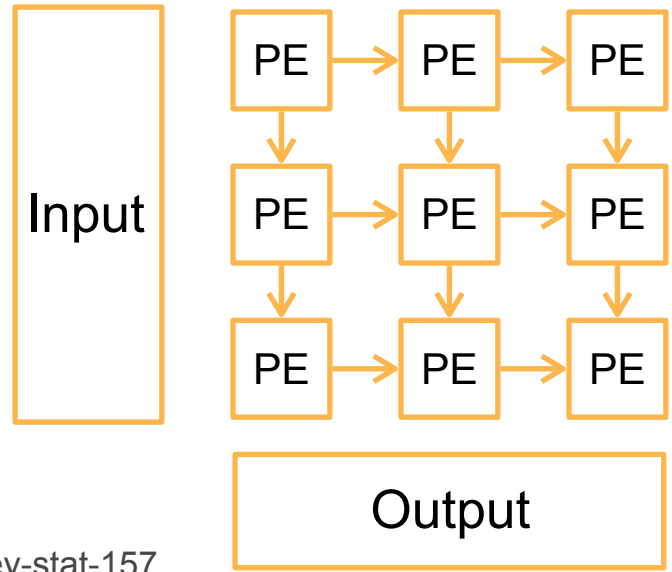
Systolic Array

- An array of processing elements (PE)
- Good at performing matrix-matrix multiplication
- Relative easy/cheaper to build



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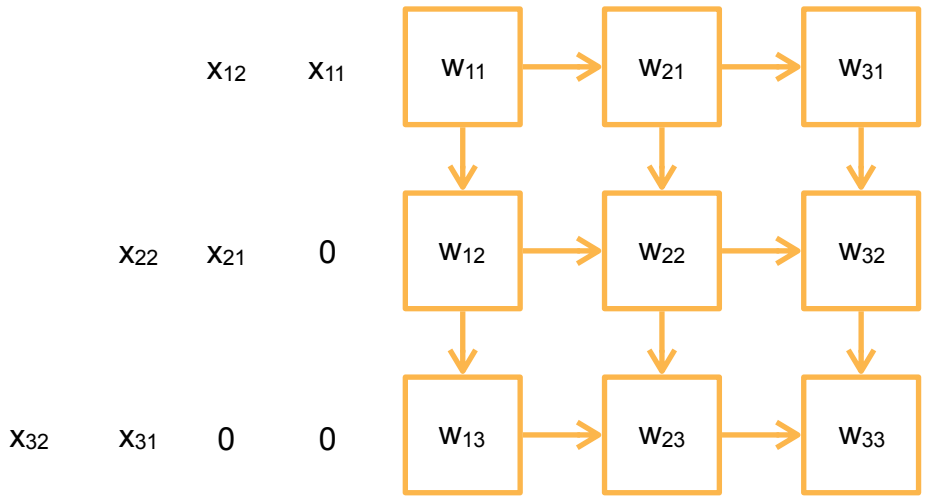
Matrix Multiplication with Systolic Array

Time 0

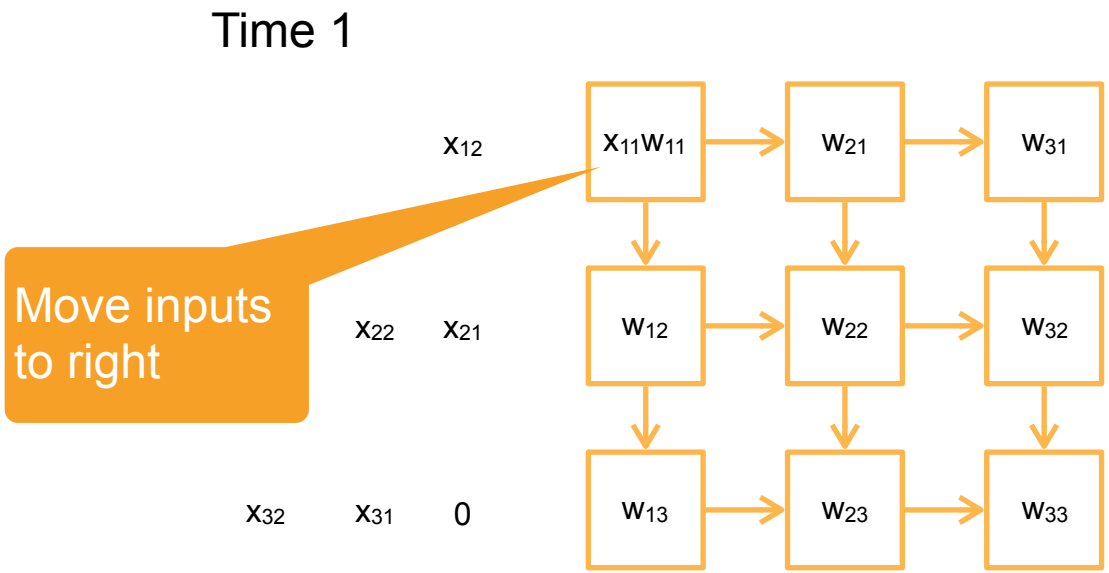


$$\mathbf{Y} = \mathbf{WX}$$

3x2 3x3 3x2

aws

Matrix Multiplication with Systolic Array

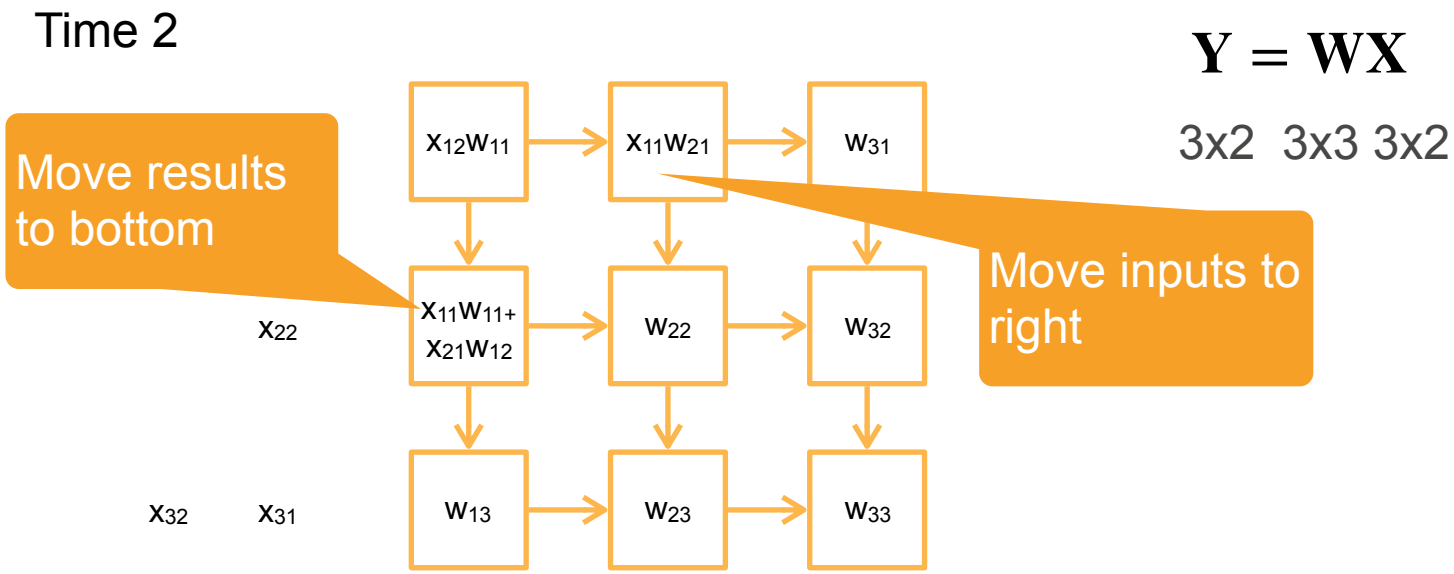


$$\mathbf{Y} = \mathbf{WX}$$

3x2 3x3 3x2

aws

Matrix Multiplication with Systolic Array

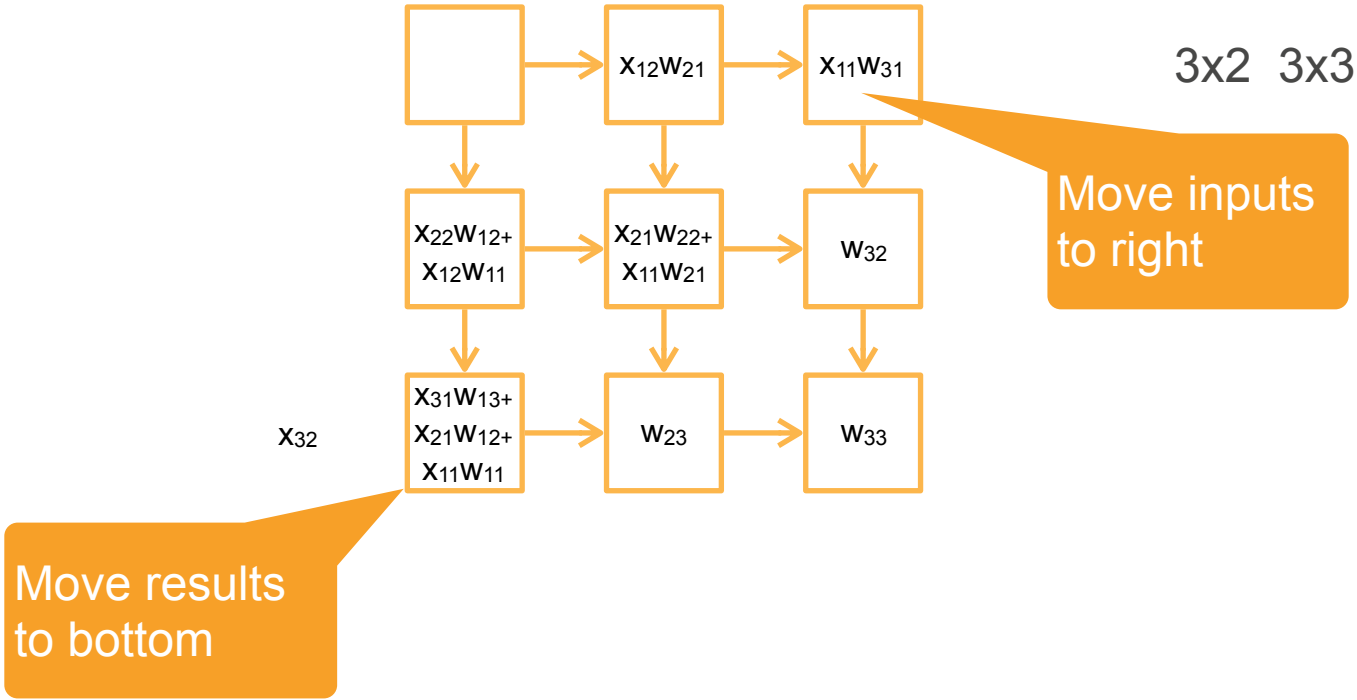


Matrix Multiplication with Systolic Array

Time 3

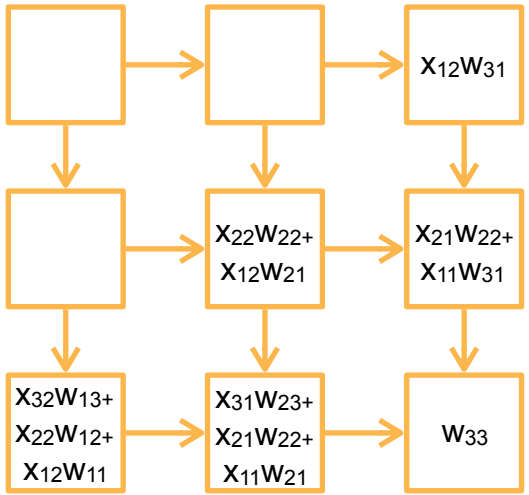
$$\mathbf{Y} = \mathbf{WX}$$

3x2 3x3 3x2



Matrix Multiplication with Systolic Array

Time 4



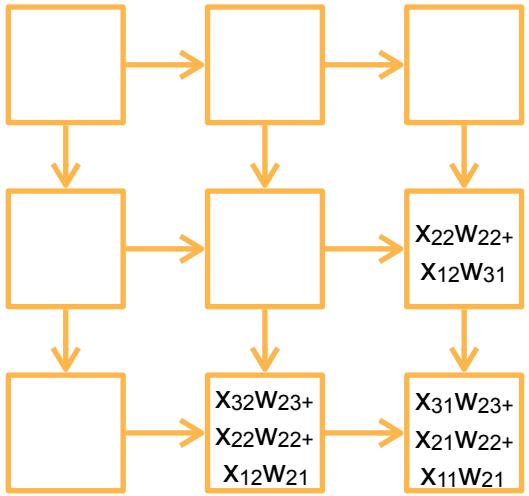
$$\mathbf{Y} = \mathbf{WX}$$

3x2 3x3 3x2

aws

Matrix Multiplication with Systolic Array

Time 5



y_{12} y_{21}

y_{11}

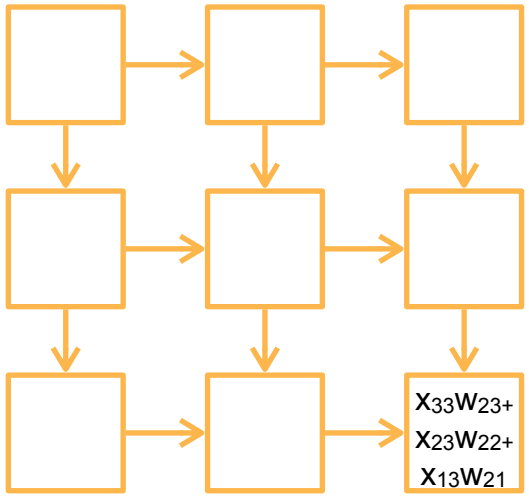
$$\mathbf{Y} = \mathbf{WX}$$

3x2 3x3 3x2

aws

Matrix Multiplication with Systolic Array

Time 6



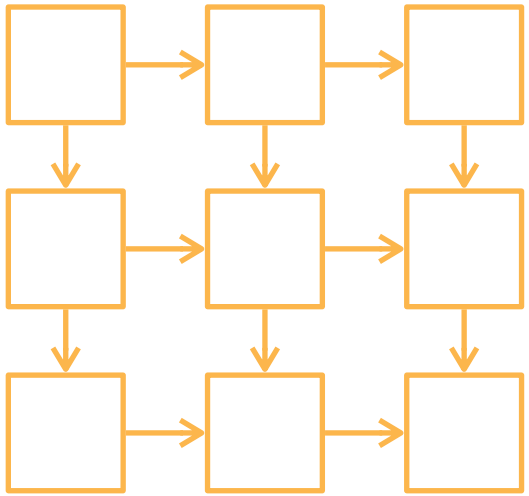
$$\mathbf{Y} = \mathbf{WX}$$

3x2 3x3 3x2

aws

Matrix Multiplication with Systolic Array

Time 7



$$\mathbf{Y} = \mathbf{WX}$$

3x2 3x3 3x2

y_{32}

y_{22} y_{31}

y_{12} y_{21}

y_{11}

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Systolic Array

- For general size matrix multiplication, slice and pad inputs to match the SA size
- Batch inputs to reduce the latency cost
- ASIC has other dedicated components for other NN operations, such as sigmoid

aws


Flexibility and Ease of Use
intel
CORE i7
7th Gen
TITAN X
Hexagon 685 DSP
Xilinx®
FPGA
Performance & Power Efficiency