

These slides have not yet  
been updated for the  
Spring 2019 semester

# Training

Arthur J. Redfern  
[arthur.redfern@utdallas.edu](mailto:arthur.redfern@utdallas.edu)

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# Outline

- Motivation
- Data
- Initialization
- Forward pass
- Error calculation
- Backward pass
- Weight update
- Evaluation
- Hyper parameter selection
- References

The 1 learning hypothesis of the brain ...

C. Metin and D. Frost, "Visual responses of neurons in somatosensory cortex of hamsters with experimentally induced retinal projections to somatosensory thalamus," PNAS Neurobiology, p. 357-361, 1986.  
-> Taught the somatosensory cortex to see in hamsters

A. Roe et. al., "Visual projections routed to the auditory pathway in ferrets: receptive fields of visual neurons in primary auditory cortex," Journal of Neuroscience, p. 3651-3664, 1992.  
-> Taught the auditory cortex to see in ferrets

# Motivation

# Parameter Estimation To Maximize Accuracy

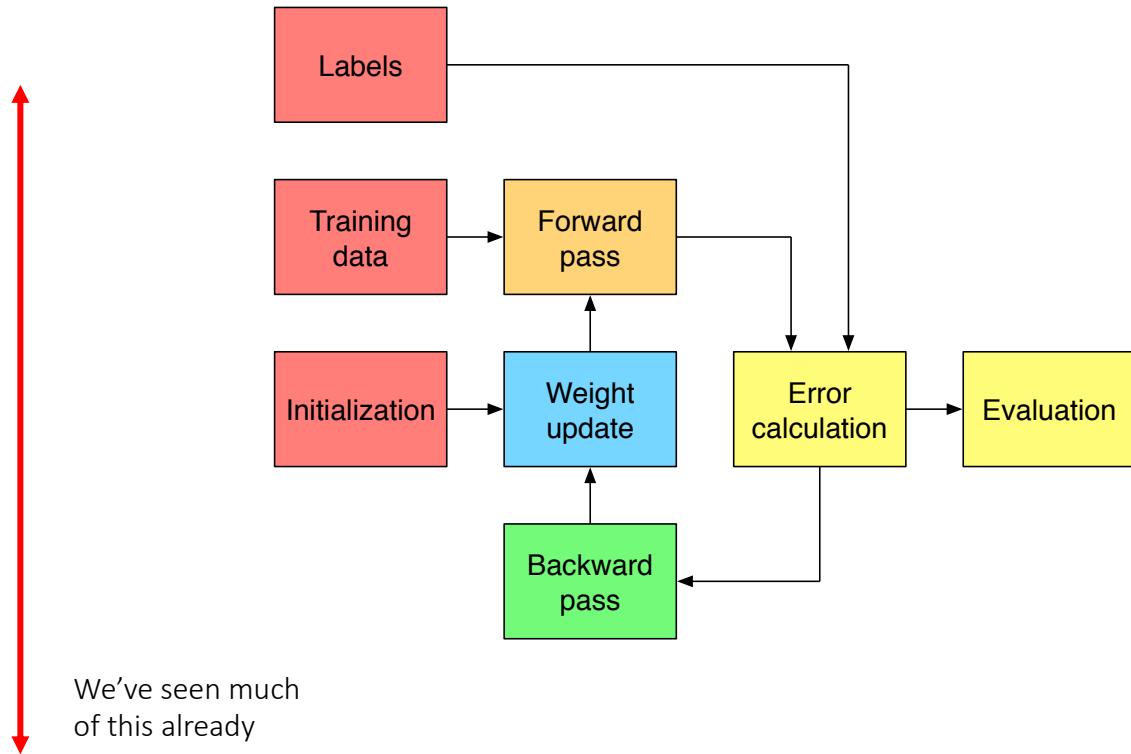
- The previous lectures looked at a lot of CNN designs
- The goal of training is to find the parameters that control the input output mapping of the (typically) linear operations in a CNN design to maximize the accuracy of the full network on testing data
- Conceptually, extracting information from training data to enable the extraction of information from testing data

Example of doing this as a human in this class

- We look at a lot of different networks, I label the different parts and describe how they work together to allow the network to do what it does
- From this you start to build knowledge in network design (training)
- You read a new paper with a new network design
- In the new paper you recognize the different parts and recognize new innovations and how they interact to allow the network to do what it does (testing)

# Supervised Learning Framework

- Hyper parameter selection
- Initialization
- Training
  - Update (serial or parallel)
    - Training data selection
    - Forward pass
    - Error calculation
    - Backward pass
    - Weight update
    - Repeat (~ batch)
  - Evaluation / validation
    - Validation data accuracy
    - Break if appropriate
  - Repeat (~ epoch)
- Testing
  - Evaluation / testing
    - Testing data accuracy



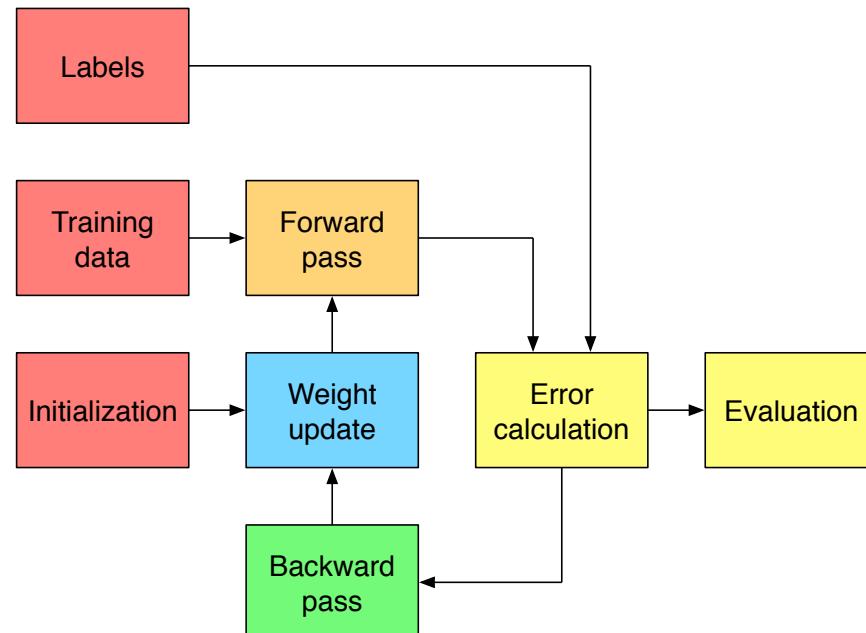
# CNN Training Vs Function Optimization

Training builds on the optimization framework discussed during the calculus lectures but there are meaningful conceptual and practical differences

- Differences

- Different data sets
- Different initialization strategies
- Forward pass modifications
- Different error calculations
- Backward pass modifications
- Different weight updates
- ...

- Will look at each of these in subsequent slides



# Overfitting Regularization And Generalization

All definitions are informal; see <https://developers.google.com/machine-learning/glossary/> for a general glossary of terms

- Generalization is the ability of a model (network) to make accurate predictions on testing data given training on training data
  - Generalization gap is the difference in accuracy of the network on training data vs testing data
  - Differences between training and optimization lead to a potential issue with generalization
- Overfitting refers to a model optimized on training data in a way that fails to nicely generalize to testing data
  - CNNs are highly parameterized models that while excellent in their universal approximation capabilities have the downside of potentially overfitting training data
- Regularization modifies training to improve generalization
  - A number of different regularization strategies will be described in subsequent sections

# Overfitting Regularization And Generalization

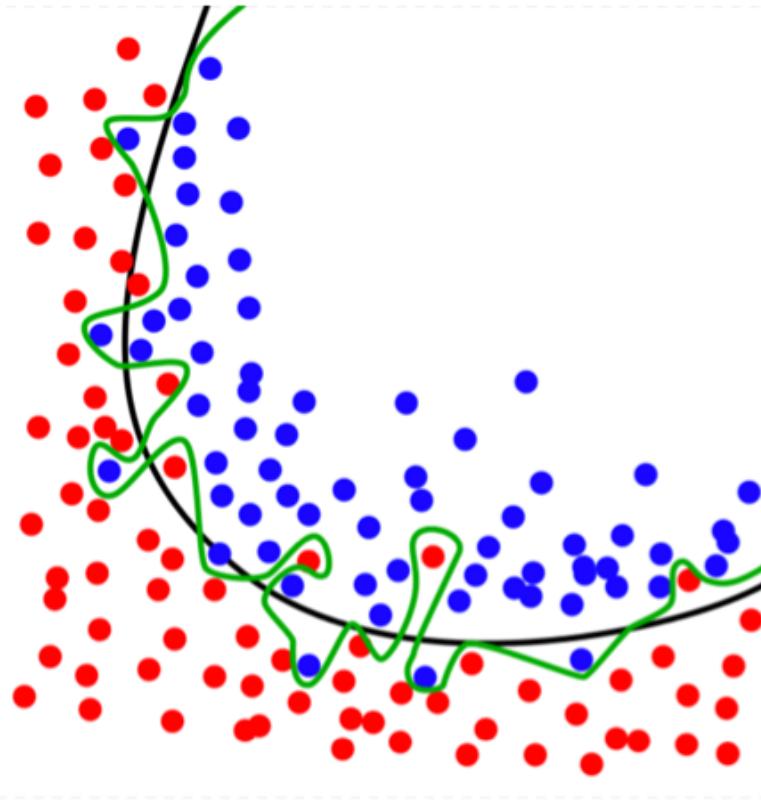
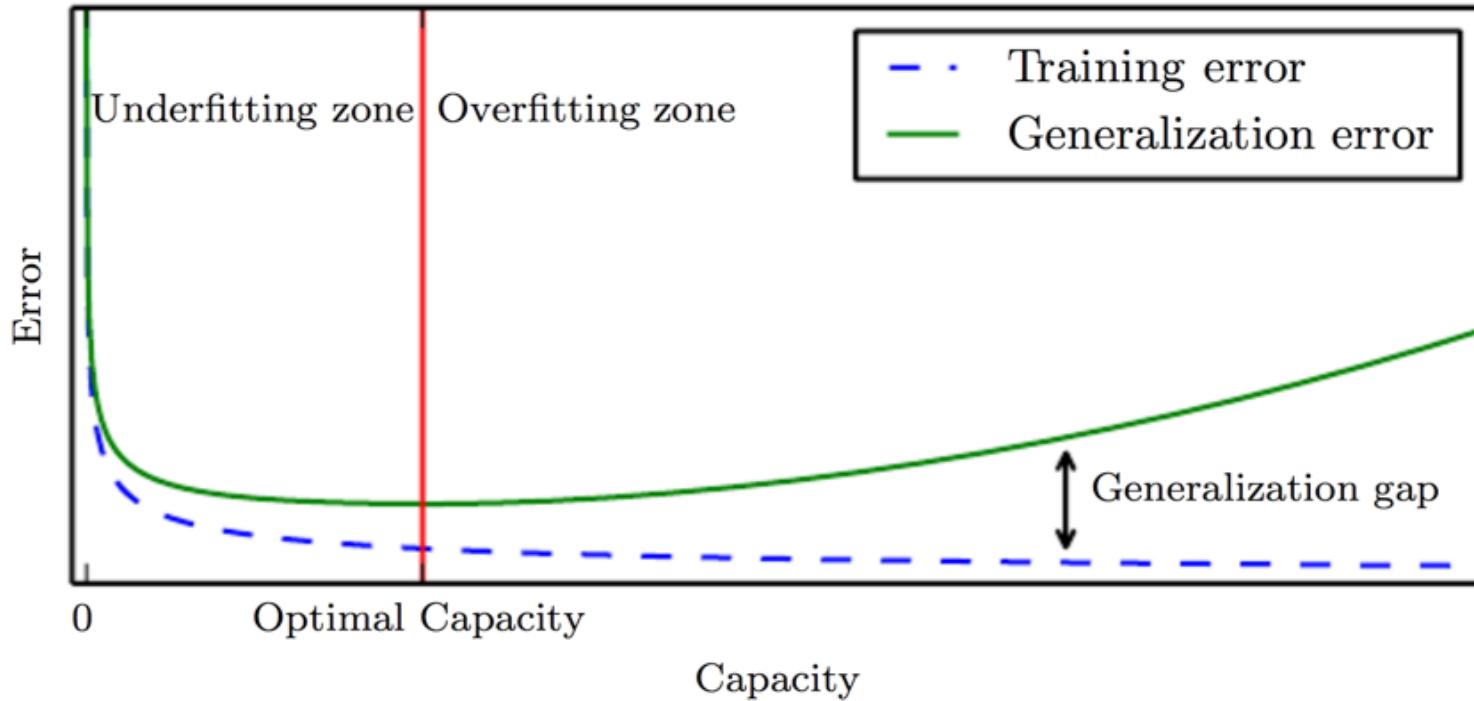


Figure from <https://en.wikipedia.org/wiki/Overfitting#/media/File:Overfitting.svg>

# Overfitting Regularization And Generalization



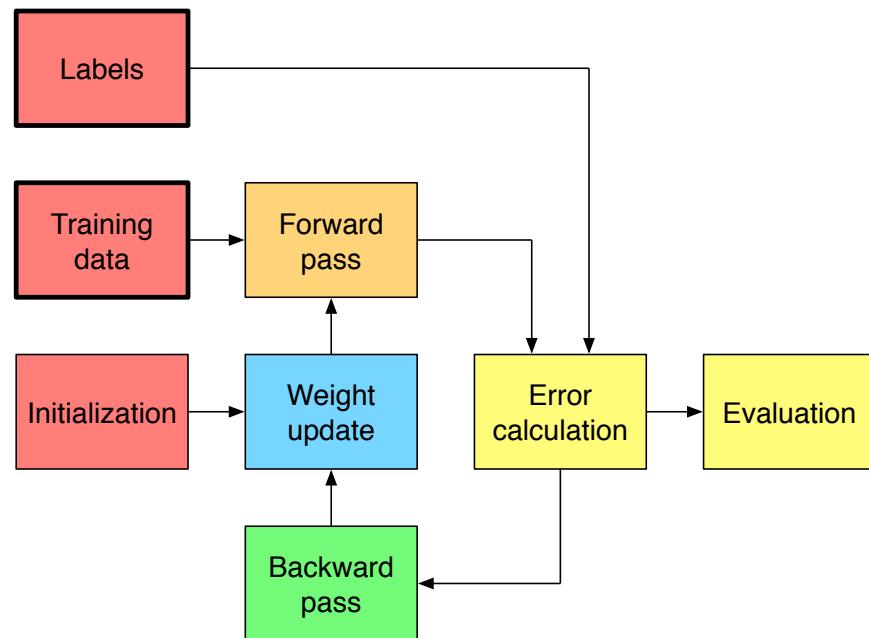
# Convergence And Generalization

- Given the previous slides, on subsequent slides you will notice methods serve 1 or more purposes
  - Improve convergence
  - Improve generalization
- Example: to improve convergence in very deep networks
  - Use optimal standard deviation during weight initialization
  - Add batch norms after convolutions
  - Use residual connections
- Keep this in the back of your mind as you continue reading

# Data

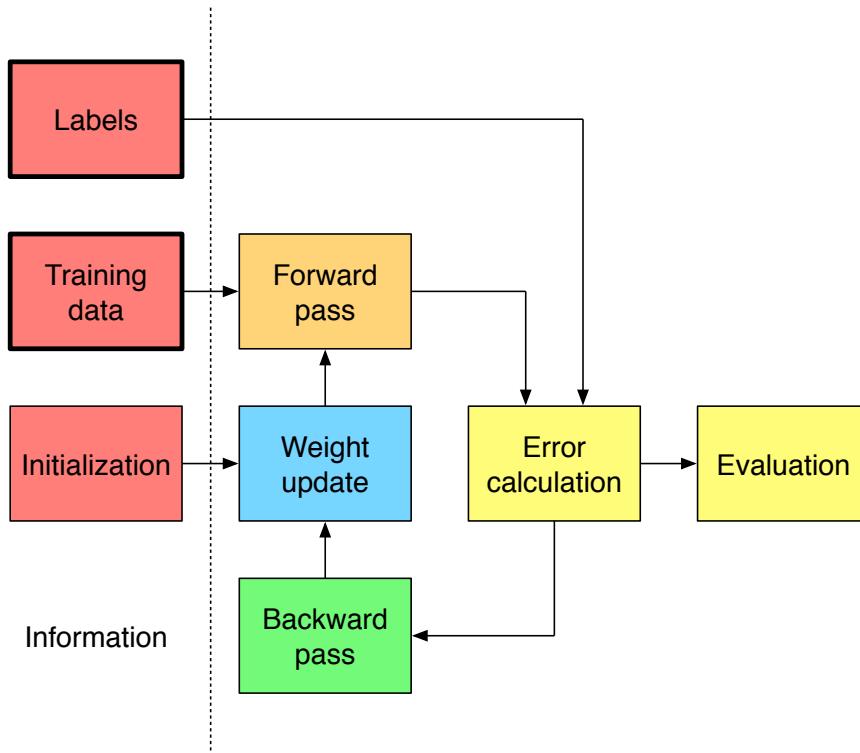
# CNN Training Vs Function Optimization

- CNN training
  - 1 data set used for training
  - Typically a different data set used for validation
  - Definitely a different data set used for testing
- Function optimization
  - Same data set used for training and optimization
  - Generalization is less of / not an issue



# Data Contains Information

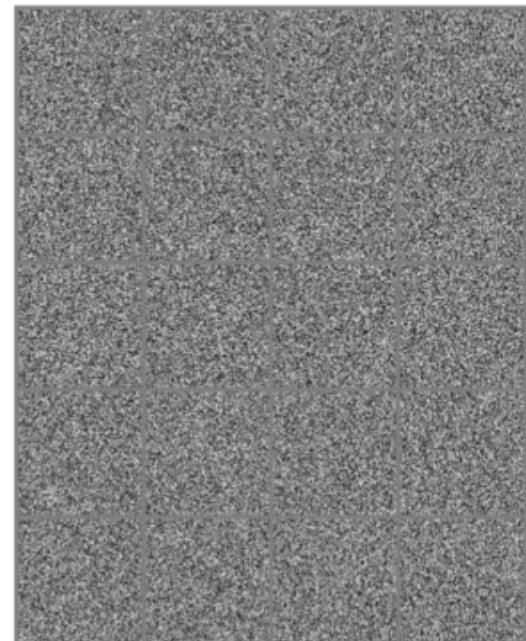
- Impossible to overstate the importance of data (really information) to learning
- For training
  - The more data the better
  - Want good representations of all possible classes / types
  - Want in as many settings as possible
  - Want as similar to the testing data as possible
- Note that initialization weights potentially also contain information (they will be discussed in the next section)



# The Curse Of Dimensionality

- The curse of dimensionality: available data for training is sparse relative to all possible data realizations
  - Consider images
  - Consider sounds
- But we can train networks using sparse training data to work on testing data for many cases that we care about: how is this possible?
  - Natural <images, sounds, ...> live on a much smaller dimensional subspace than all possible
  - Successful applications of machine learning are likely possible because of this
  - Frequently exploited via some time, space, spatial frequency, ... in the data

20 random images  
(that look nothing like natural images)



Question: how many different possible 8 bit images of size  $3 \times 1024 \times 2048$  are there? Note:  $256^{6000000}$  is a big number

# Training | Validation | Testing Data Split

- Reminder: training data  $\cap$  testing data =  $\emptyset$ 
  - Train on training data
  - Test on testing data
- Training and validation data
  - Training data is used for weight updates
  - Validation data is used to periodically monitor progress during training
  - Typical strategy: split training data into training data and validation data
  - Variations on a theme (amount of split, what data to include where, ...)
- Testing data
  - Use to estimate final performance
  - Hidden danger: repeated passes through the flow make effectively make testing data part of training data
  - This is a very real problem for xNNs with lots of parameters and testing many different network and / or training configurations

## CNNs vs other ML methods

- It's common in many machine learning training methods to have a small amount of training data and do cross validation (over repeated trials choose different partitions of the training data for training and validation)
- 1 problem with this for CNNs is that CNNs typically don't train well with a small amount of data
- Another problem is that the high capacity of CNNs makes memorization possible which hurts the use of validation data for determining when to stop training
- This is related to the hidden danger mentioned under testing data

# 2 Classes Of Training Data

Natural



Synthetic



# Natural Data

- Natural data takes advantage of nature's data generation process
  - Doesn't require information on our part
  - Nature supplies the intelligence
  - Natural as used here applies to data generated or measured from a physical environment by a person
  - Ex: images, sounds, radar, lidar, ultrasound, EEG, ...
- It's nice if there's relative uniformity of data generated by different sensors of the same type
  - This allows for training data taken from 1 sensor to be used to train weights for a network that processes a different sensor
  - It typically implies that the data can be transformed to a common representation (e.g., image sensor and an ISP)
  - Different sensor types can have different common representation (e.g., maybe a RGB image for an image sensor vs a point cloud for a radar)
- A challenge is labeling
  - The number of samples needed for training large network is large
  - Potentially the complexity of labeling even a single sample is high

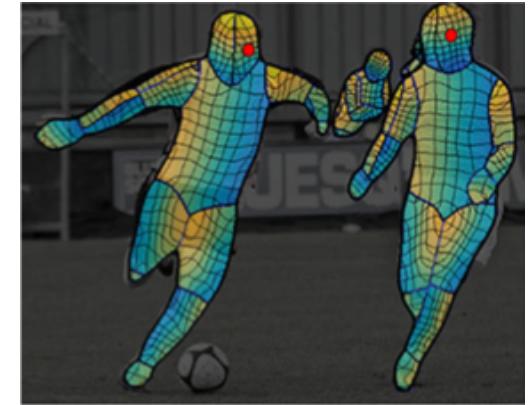
# Labeling Data (Is Miserable)

- CNNs like lots of data for training
- The complexity of labeling a single sample can vary a lot
  - Easy
    - 1 input 1 label a few classes
  - Moderate
    - 1 input 1 label many classes
  - Hard
    - 1 input many labels
    - Common to build tools to help
    - Streamline the labeling process
  - Impossible (-ish)
    - Depth after the fact



# Labeling Data (Is Still Miserable)

- CNNs like lots of data for training
- The complexity of labeling a single sample can vary a lot
  - Easy
    - 1 input 1 label a few classes
  - Moderate
    - 1 input 1 label many classes
  - Hard
    - 1 input many labels
    - Common to build tools to help
    - Streamline the labeling process
  - Impossible (-ish)
    - Depth after the fact



# Tools Money Deception And Coercion

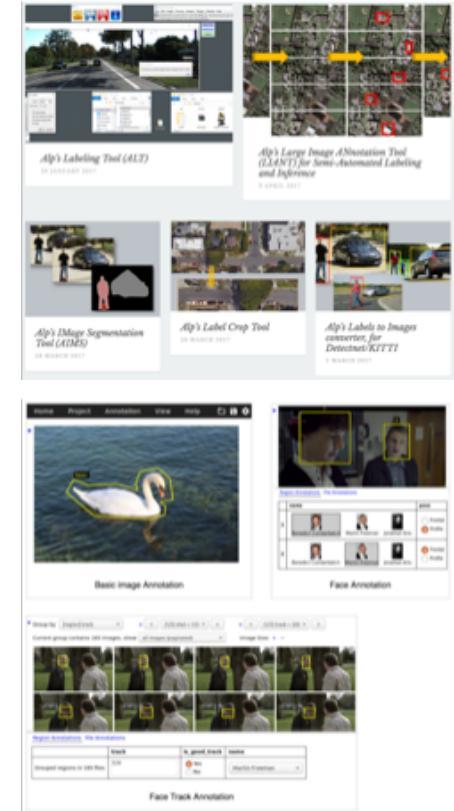
- In practice, build tools then use tools + humans to label
- How to get humans to label
  - Pay people (Mechanical Turk)
  - Coerce people (grad students, relatives)
  - Figure out a way of getting people to do it even though they don't realize they are (games, apps)
  - Realize it's not getting done as fast as you'd like and do it yourself



Amazon Mechanical Turk (MTurk) operates a marketplace for work that requires human intelligence. The MTurk web service enables companies to programmatically access this marketplace and a diverse, on-demand workforce. Developers can leverage this service to build human intelligence directly into their applications.

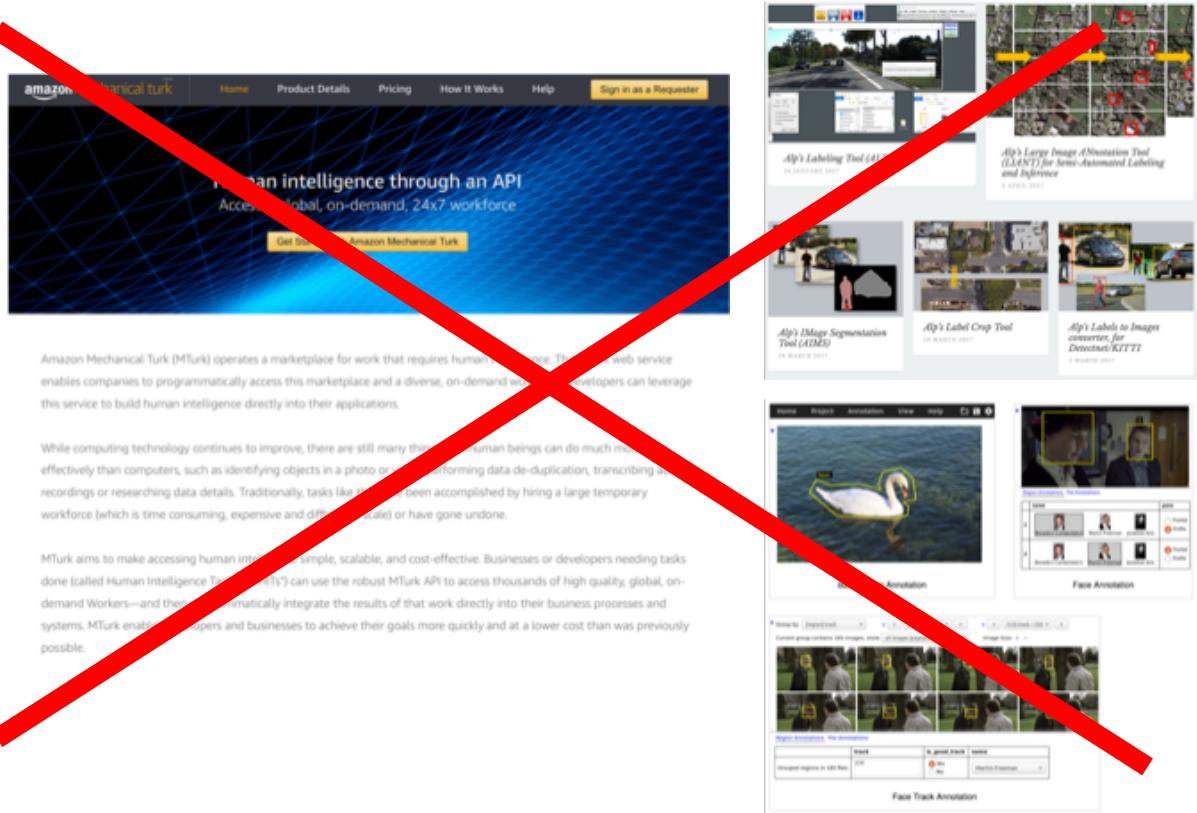
While computing technology continues to improve, there are still many things that human beings can do much more effectively than computers, such as identifying objects in a photo or video, performing data de-duplication, transcribing audio recordings or researching data details. Traditionally, tasks like this have been accomplished by hiring a large temporary workforce (which is time consuming, expensive and difficult to scale) or have gone undone.

MTurk aims to make accessing human intelligence simple, scalable, and cost-effective. Businesses or developers needing tasks done (called Human Intelligence Tasks or "HITs") can use the robust MTurk API to access thousands of high quality, global, on-demand Workers—and then programmatically integrate the results of that work directly into their business processes and systems. MTurk enables developers and businesses to achieve their goals more quickly and at a lower cost than was previously possible.



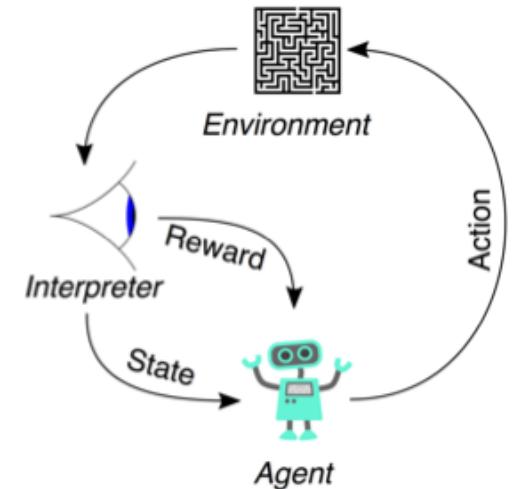
# The Dream

- The dream: training CNNs with unlabeled data (unsupervised learning)
  - There's usually orders of magnitude more unlabeled data than labeled data
- The reality: training CNNs tends to work a lot better with labeled data (supervised learning)
- Likely some tradeoff / information balance between unsupervised and supervised learning
  - Less data (information) + labels (information)
  - More data (information) but no labels



# Somewhere In Between ...

- ... unsupervised and supervised learning lies ...
- Semi supervised learning (some labeled data, some unlabeled data)
  - Example: train multiple CNNs with labeled training data using supervised learning
  - Use unlabeled data as an input and treat the ensemble output label as the correct label
  - Use the ensemble output label with supervised learning to update the individual CNNs
- Reinforcement learning
  - From the current state an agent chooses an action and the environment provides a reward and new state; the combination of input {current state, action} and output {reward, new state} can be used to generate an error signal
  - But the output is frequently sort of 1 step removed from a label (e.g., what really is the value of the new position); so the information content in the output is typically not as strong as the supervised learning cases
  - As such, most reinforcement successes are linked to cases where huge amounts of simulated input output pairs are possible to test and smart strategies are used to approximate labels



Note: will discuss reinforcement learning more in the context of games

# Cleaning

- If data is incorrectly labeled then training on it can negatively impact testing accuracy
- Cleaning: remove bad data
- Examples
  - Multiple people labeling the same data
  - 0 lag tick filtering (reminder: tell story)

$$E = mc^3$$

(if you were a physics student and learned this it would likely negatively impact your testing accuracy, i.e., grade; xNNs are no different)

# Examples

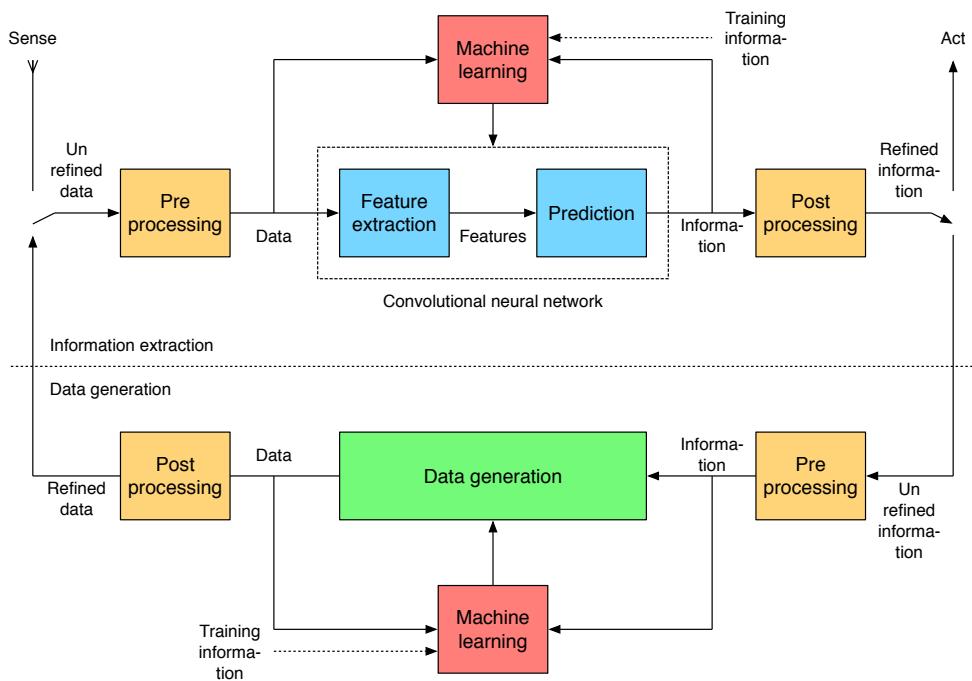
- Labeled classification datasets were created 1st for vision
  - Easiest task to outsource (e.g. Amazon Mechanical Turk)
  - Largest public dataset: ImageNet (1.2M images, 1000 classes)
  - Largest private dataset (that I know about): JFT (100M images, 15k classes)
- Pixel wise labeling can be very expensive
  - Segmentation example: Daimler Cityscapes
    - Fine annotations (5,000 images @ 90+ min each)
    - Coarse annotations (20,000 images @ 7 min each)
    - Total time: 9833 hours (24.5 weeks w / 10 full time people)
  - Other examples: depth, motion, ...
- Examples datasets for vision
  - MNIST, CIFAR 10 / 100, ImageNet, Pascal VOC, KITTI, COCO, Cityscapes, ...



Images from Microsoft COCO  
<http://cocodataset.org/>

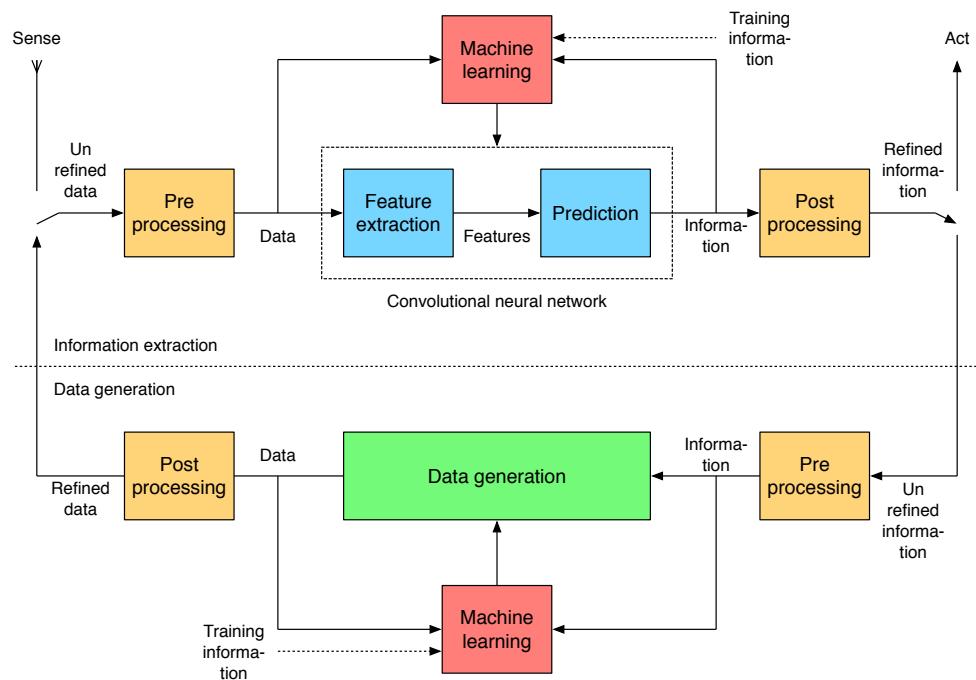
# Synthetic Data

- Reminder
  - Introduction lecture mentioned that there are 2 types of problems
  - Data to information (basically everything we've talked about so far)
  - Information to data (relevant here among other places)
- Thinking
  - Labeling data is miserable
  - So instead invert the problem
    - Which may or may not be easier
  - Synthetic data: start from a label and use an algorithm to generate associated data
  - The data / label combination can then be used for supervised training



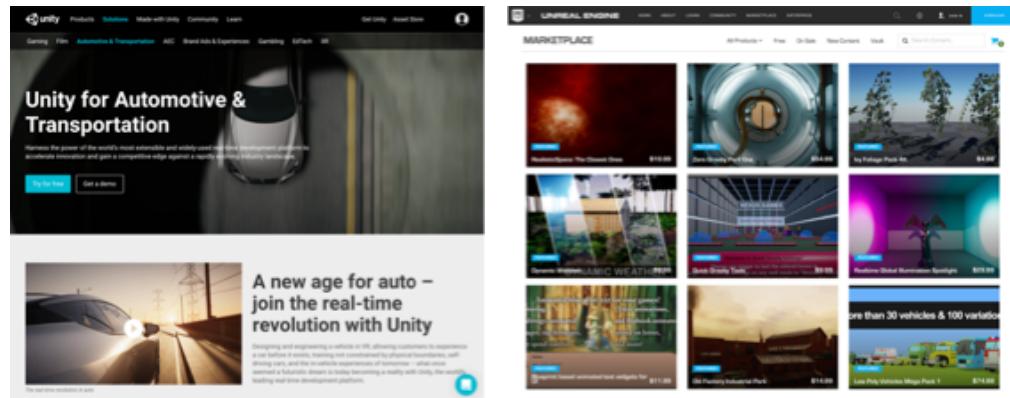
# 2 Ways To Generate Synthetic Data

- Reminder
  - When we talked about methods for going from data to information there were 2 basic categories
    - Hand engineered
    - Learned
  - The same applies to going the other direction from information to data
- Hand engineered
  - Requires intelligence on our part
  - Ex: computer vision (thank you to the video game and movie special effects industries)
- Learned
  - Extracts knowledge from nature's information to data generation process to train an algorithm to generate data from information



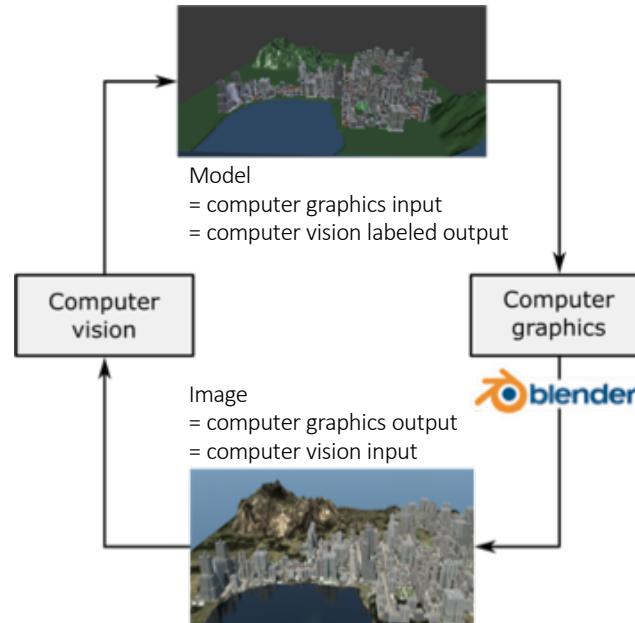
# Hand Engineered

- The information content of the generated synthetic data is limited by the information content of the hand engineered model used to generate the data (but for some cases this is a lot)
- Examples
  - Computer graphics



# Computer Graphics

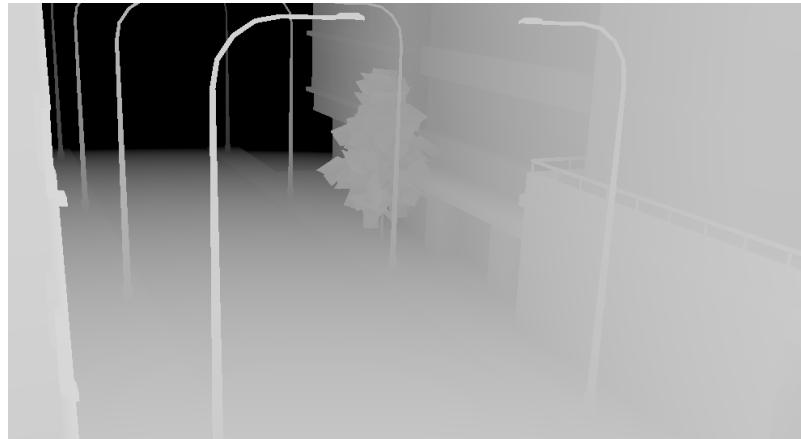
- Computer graphics and computer vision are the opposites (cousins?) of each other
  - We can take advantage of advances in computer graphics from gaming, ... to generate realistic synthetic data
- Example uses
  - RGB images with lenses (industry standard, fisheye warped, ...) and orientations (surround, stereo, ...)
  - Depth and motion
  - Semantic and instance segmentation
  - Events in different conditions and unlikely events



# Synthetic Depth Data



Rendered image



Labeled depth

Example RGB and depth renderings

Dense depth labels are difficult to obtain in practice (e.g., KITTI is ~30% labeled)

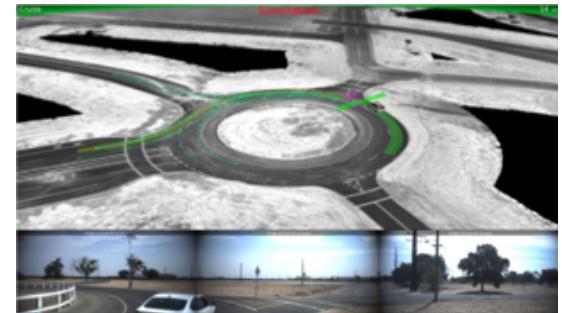
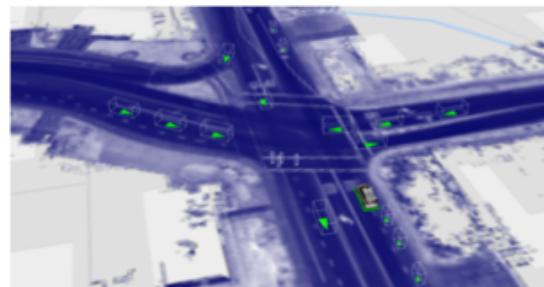
# Synthetic Virtual KITTI Data



Virtual worlds as a proxy for multiple-object tracking analysis  
(<https://arxiv.org/abs/1605.06457>)

# Synthetic Carcraft Data

- Google / Waymo Carcraft
  - > 8 million virtual miles driven per day
  - > 2.5 billion virtual miles driven total

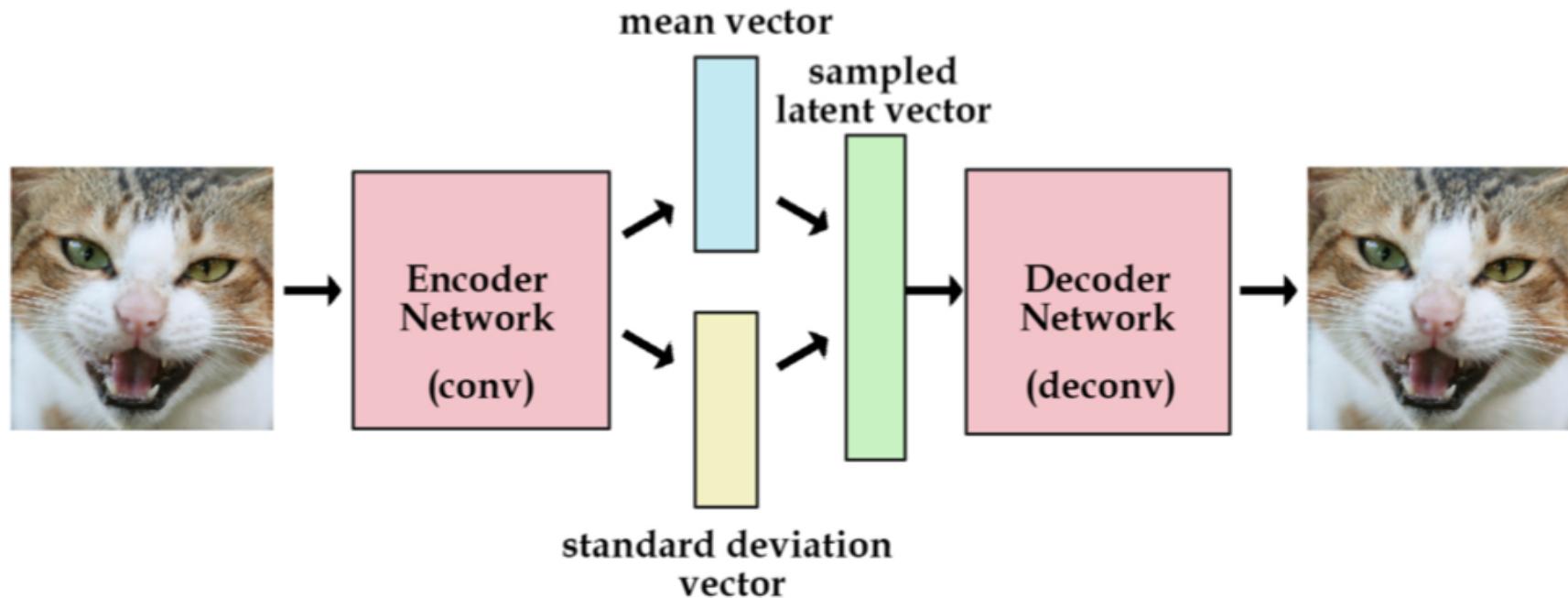


Images from <https://www.theatlantic.com/technology/archive/2017/08/inside-waymos-secret-testing-and-simulation-facilities/537648/>

# Learned

- Thought chain
  - Neural networks provide a structure for learning to map from data to information
  - So instead of a hand engineered mapping, is it possible to train a neural network to learn to map from information to data (i.e., the other direction)?
  - Subtlety: The information content of the generated synthetic data is limited by the information content of data used for training the algorithm for generating the data
- An auto encoder is an example structure that learns to recreate its input after its input is pushed through a bottleneck
  - The bottleneck forces a representation that contains the key underlying features of the data
  - Can then start at the bottleneck and generate new data (e.g., see variational auto encoder)
- A generative adversarial network is an example that learns a generative model that generates examples similar to the characteristics of natural samples
  - Typically learned in conjunction with another algorithm for information extraction that determines if data is natural or synthetic

# Variational Auto Encoder



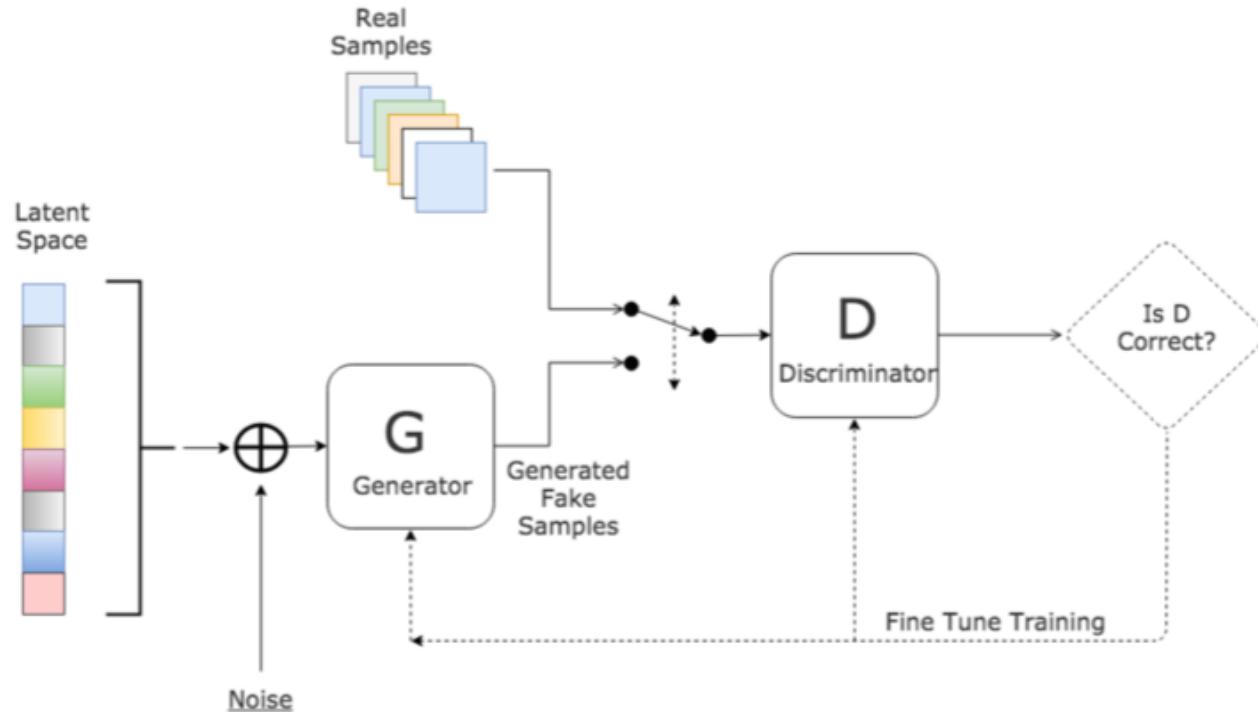
Variational autoencoders explained (<http://kvfrans.com/variational-autoencoders-explained/>)

# Variational Auto Encoder



Auto-encoding variational bayes (<https://arxiv.org/abs/1312.6114>)

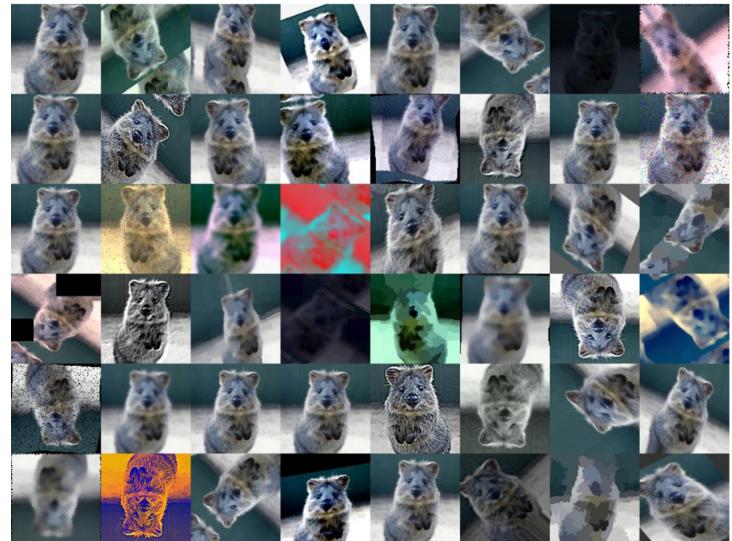
# Generative Adversarial Networks



Note:  
there's a lot  
of activity in  
this area  
and this  
topic may  
get it's own  
focused  
lecture later  
in the  
semester

# Data Augmentation

- Basically always want more data to improve training
  - Generate new data by augmenting existing data via modifications
  - Target places where training data is insufficient for learning to achieve a desired level of accuracy on testing data
- Starting point can be real or synthetic data
  - Augmentation can be abstract
    - Warping, flips, color distortions, additive noise, ...
  - Augmentation can be meaningful
    - Changing time of day or weather
- The amount of information added is based on the augmentation process
  - Even if 0 (e.g., noise or a deterministic invertible mapping) it's still potentially useful to training if it helps regularize the learning process



# Synthetic Virtual KITTI Data

Clone



Overcast



Fog



Rain



Morning

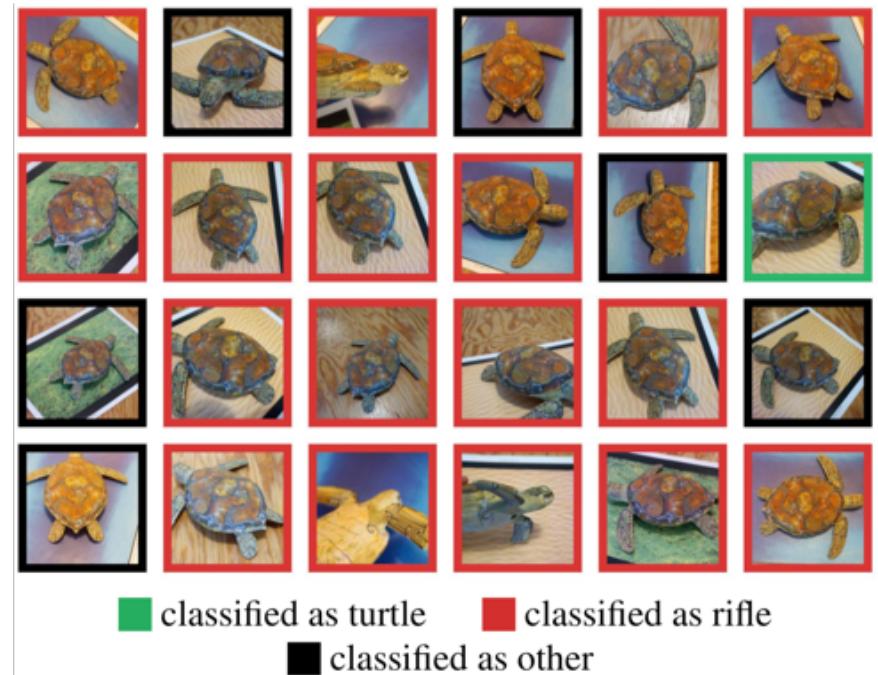


Sunset



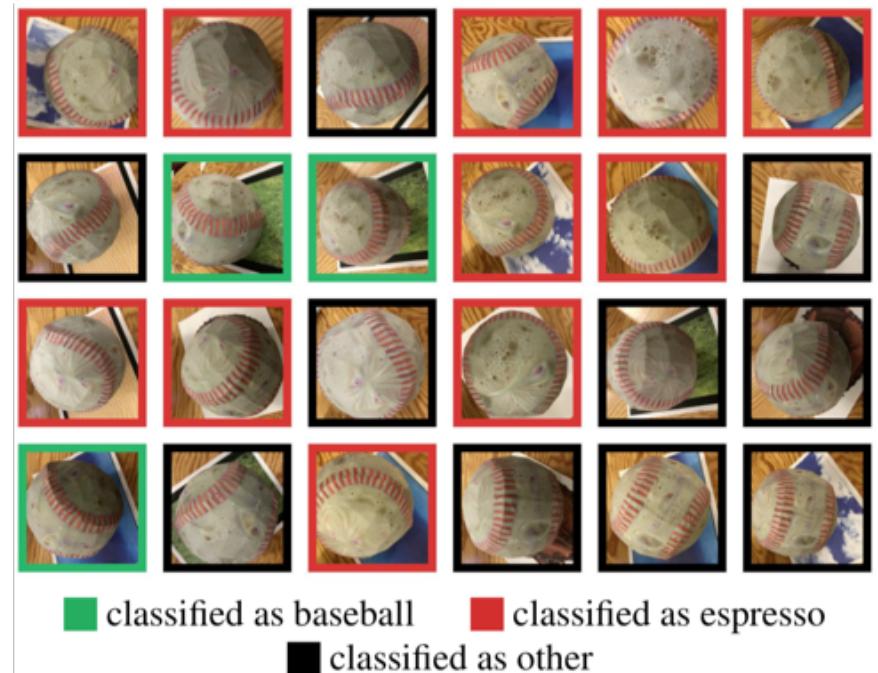
# Adversarial Examples

- High capacity networks that map from data to 1 of many classes can be easily fooled
  - An input that humans are confident in correctly classifying that looks like a typical member of a class
  - But a network is confident in incorrectly classifying to a totally different class
- These types of inputs are called adversarial
- Why create adversarial examples?
  - The good: to use as a data augmentation method for generating additional training samples to make a network more robust
  - The bad: to fool a network into making an incorrect decision for a negative purpose



# Generating Adversarial Examples

- Goal: generate examples with the following characteristics
  - Human strongly believes generated data belongs to class A
  - Information extraction algorithm strongly believes generated data belongs to class B
- Strategy
  - Input natural image from class A
  - Input information extraction algorithm
  - Input human perception sensitivity information
  - Use optimization algorithm to compute perturbation of natural image from class A based on the information extraction algorithm and human perception sensitivity that achieves the goals



# Selecting Samples Of Training Data

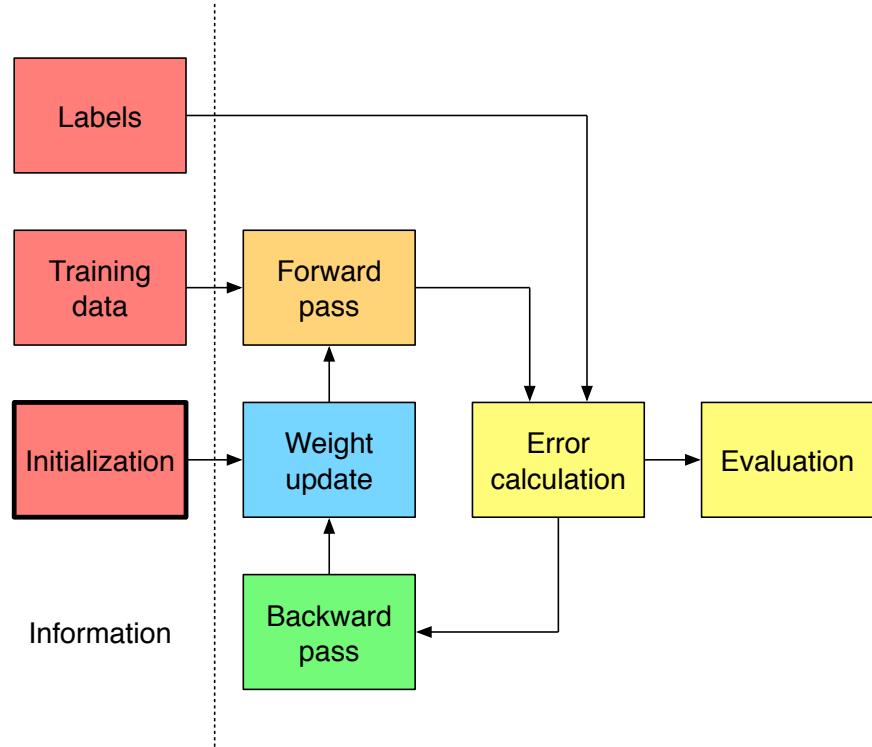
- Batch / iteration / epoch
  - Batch size: a group of inputs (a batch) used to make a single weight update
  - Number of iterations: number of weight updates
  - Number of epochs: batch size \* number of iterations / number of training samples
- Options for selecting training samples
  - Walk through a random ordering of all training data a batch at a time
  - Start with easier samples then move to harder samples (curriculum learning)
  - Force some level of balance in different samples
  - Force some bias in different samples
  - More difficult cases vs easy cases (online hard example mining)
  - For subsequent epochs can keep the same ordering or switch to a new random ordering (sometimes a hassle due to practical data preparation constraints)
  - ...

Batch size will be discussed more during the weight update section

# Initialization

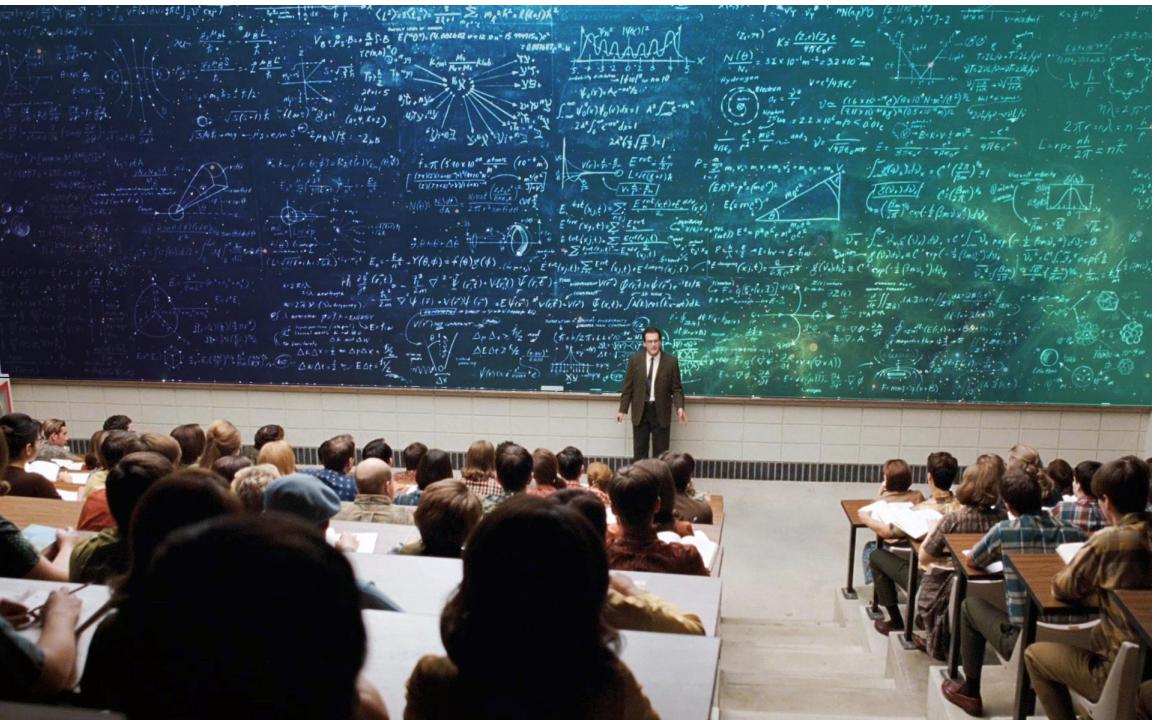
# Strategies

- Random initialization
  - When you only know things probabilistically
- Transfer learning
  - From a different problem
  - From a simpler version of the same problem (curriculum learning)



# Random Initialization

- Training a model “from scratch”
- Typically use random initialization
  - Don’t choose all zeros
  - Do use multiple probably independent realizations of a random variable
  - Maybe handle weights different than biases
- Need to determine
  - Distribution type
  - Mean, variance, ...

Figure from <http://radscreens.com/i/9709/> 43

# How To Compute $2^{1/2}$ In 5th Grade

- Algorithm

- $x = 2^{1/2}$
- $x^2 = 2$
- $0 = x^2 - 2$
- $0 = -\alpha(x^2 - 2)$
- $X \leftarrow x - \alpha(x^2 - 2)$

- Comment

- Ideally, you'd like to choose an initialization that's close and in a contractive basin around the true value
- Practically, when in a million dimensions with a non convex cost function, you're happy to choose a starting point that doesn't lead to divergence

Let  $\alpha = 0.1$  and  $x_0 = 1.50$

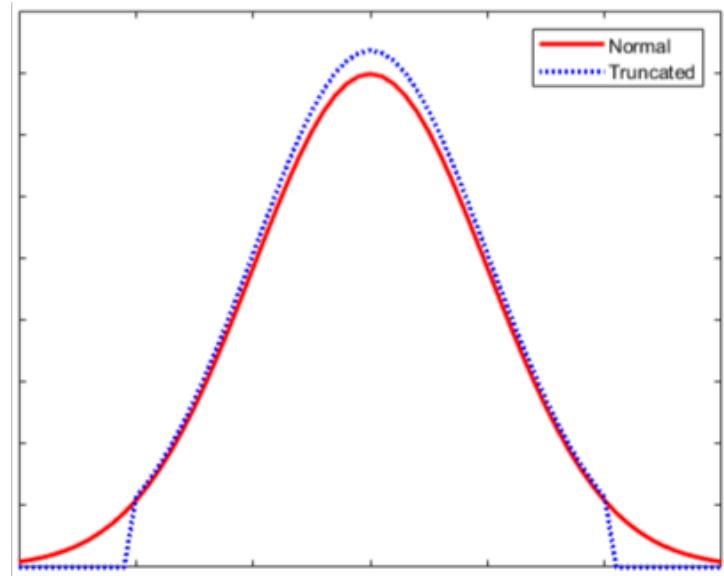
$$\begin{aligned}x_1 &= 1.48 \\x_2 &= 1.46 \\x_3 &= 1.45 \\x_4 &= 1.44 \\&\dots\end{aligned}$$

Let  $\alpha = 0.1$  and  $x_0 = 15$

$$\begin{aligned}x_1 &= -7 \\x_2 &= -12 \\x_3 &= -28 \\x_4 &= -104 \\&\dots\end{aligned}$$

# Info Theory And Distribution Choice

- What does selecting a Gaussian distribution mean from an information theoretic perspective?
  - Max entropy distribution when only the mean and variance are known
- What does selecting a uniform distribution mean from an information theoretic perspective?
  - Max entropy distribution when only the domain of support is known
- Question: which is the correct / best choice?
  - What distribution do trained models tend to follow?



# Mean = 0, Standard Deviation = ?

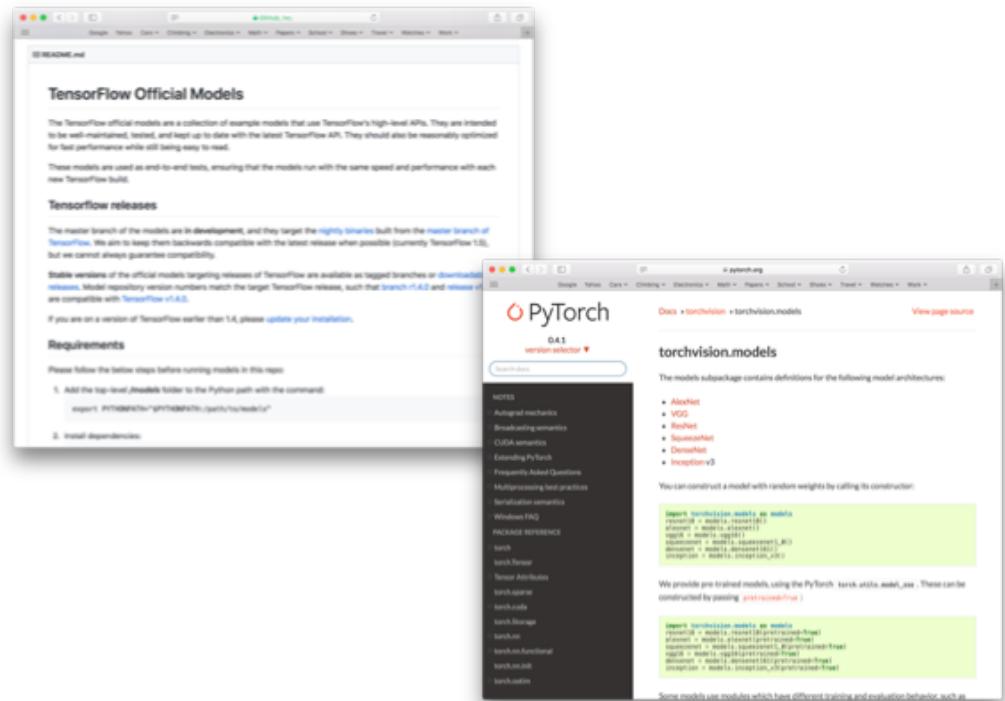
- Understanding the difficulty of training deep feedforward neural networks
  - <http://proceedings.mlr.press/v9/glorot10a.html>
  - Derived a distribution referred based on an assumption of linear activations and no exploding or vanishing data
  - Glorot / Xavier uniform:  $[-\text{limit}, \text{limit}]$  where  $\text{limit} = \sqrt{6}/(\text{fan\_in} + \text{fan\_out})$  and fan\_in and fan\_out are the number of input and output units in the weight tensor (paper is for NN, for CNN unclear if fan\_in =  $N_i * F_r * F_c$  or  $N_i$  and fan\_out = 1 or  $N_o$ )
  - Glorot / Xavier Gaussian: 0 mean and stddev =  $\sqrt{2}/(\text{fan\_in} + \text{fan\_out})$
- Delving deep into rectifiers: surpassing human-level performance on ImageNet classification
  - <https://arxiv.org/abs/1502.01852>
  - Follow a similar derivation strategy as Xavier but take the nonlinearity into account and target keeping magnitudes of inputs constant (no exponential growth or shrink of signals)
  - He uniform:  $[-\text{limit}, \text{limit}]$  where  $\text{limit} = \sqrt{6}/(F_r * F_c * N_i)$
  - He Gaussian: 0 mean and standard deviation  $\sqrt{2}/(F_r * F_c * N_i)$  and biases initialized to 0 (per paper)

# Transfer Learning

- Strategy
  - Train the network on a related problem that typically has a lot of data
  - Use those trained parameters as the starting point for the network applied to the problem of interest which typically has less data
  - May need to modify the network head to account for the differences in the problem
- How transferable are features in deep neural networks?
  - <https://arxiv.org/pdf/1411.1792.pdf>
- Can also use a smaller network to initialize a larger network or a larger network to initialize a smaller network
  - Very deep convolutional networks for large-scale image recognition
    - <https://arxiv.org/abs/1409.1556>
  - Used a strategy to train a smaller model to initialize a larger model
  - While it helps in some cases, it requires extra training and potentially has issues with getting stuck in sub optimal local minima

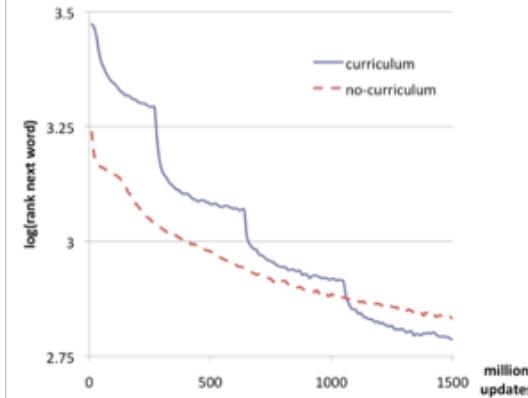
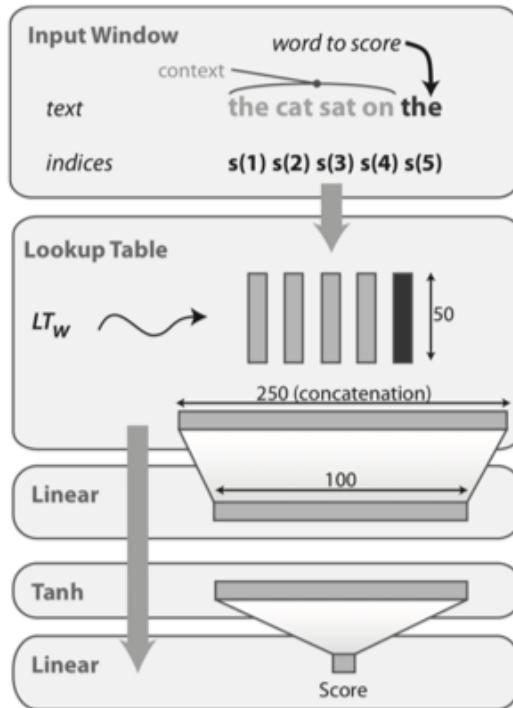
# How This Impacts You This Semester

- Training a ~ large model like ResNet 50 on ImageNet using a fast gaming system with 2x Nvidia GTX 1080 Ti GPUs can easily take a couple of weeks to a month
  - And it's very easy to mess up and have to experiment a few times with hyper parameters to get it to work
- Transfer learning let's you take advantage of the work someone else did training the network to give you a jump start as you apply it to a different but related enough problem



# Curriculum Learning

- This sits 1/2 way between the data and initialization sections
- Strategy
  - Mimic how humans learn and orders training samples typically from easier to more difficult
  - Potentially improves accuracy and generalization
  - So it's a data selection method
  - But training on easier samples can be thought of as an initialization for subsequent training on more complex samples

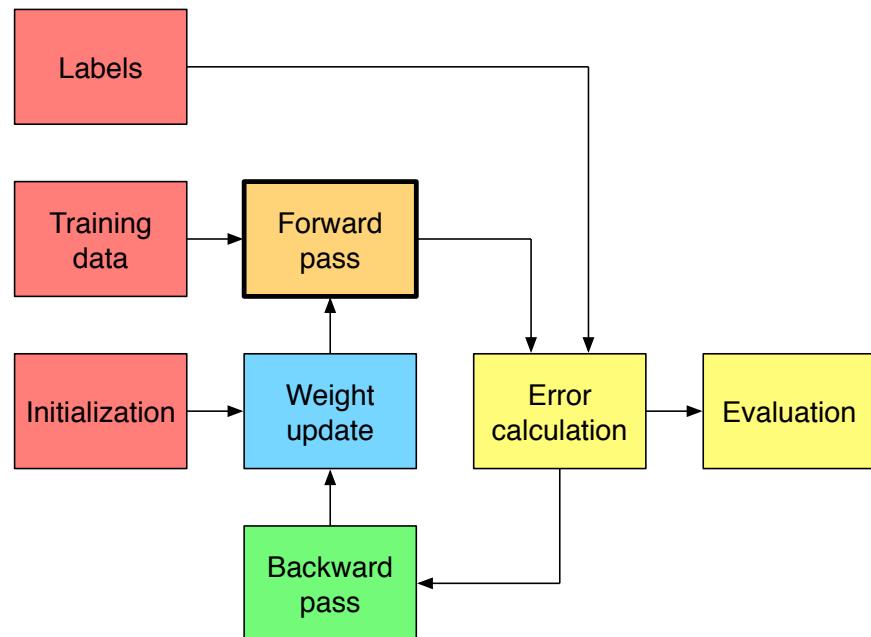


Curriculum learning  
[\(https://ronan.collobert.com/pub/matos/2009\\_curriculum\\_icml.pdf\)](https://ronan.collobert.com/pub/matos/2009_curriculum_icml.pdf)

# Forward Pass

# CNN Training Vs Function Optimization

- Modifications to the forward pass for 2 reasons
  - Convergence: improve parameter estimation on training data
  - Regularization: improve performance on testing data



# Convergence

- Strategy
  - Modify the network structure (forward pass) to improve convergence during training (backward pass)
  - After training, the network structure modification can frequently be absorbed into the original network
- Examples
  - Batch normalization
  - Batch renormalization
  - Group normalization

# Batch Normalization

- Notes
  - Initialization played all sorts of games to prevent exploding or vanishing signals as they propagate through the network
  - Idea: why not add a data dependent layer after convolution that on a per channel basis normalizes the data to 0 mean unit variance?
  - The benefits of this were described in the paper Efficient backprop (<http://yann.lecun.com/exdb/publis/pdf/lecun-98b.pdf>)
  - Note that the addition of this layer does not increase the set of functions the network can approximate in the forward path, it only improves training
- Batch normalization
  - For each batch compute a per channel mean and variance
  - Normalize each channel to  $\sim 0$  mean  $\sim 1$  variance
  - Includes learnable scale and shift parameters to maintain expressiveness in transformation
  - If possible absorb the scale and shift parameters into a neighboring layer during testing

**Input:** Values of  $x$  over a mini-batch:  $\mathcal{B} = \{x_{1\dots m}\}$ ;

Parameters to be learned:  $\gamma, \beta$

**Output:**  $\{y_i = \text{BN}_{\gamma, \beta}(x_i)\}$

$$\mu_{\mathcal{B}} \leftarrow \frac{1}{m} \sum_{i=1}^m x_i \quad // \text{mini-batch mean}$$

$$\sigma_{\mathcal{B}}^2 \leftarrow \frac{1}{m} \sum_{i=1}^m (x_i - \mu_{\mathcal{B}})^2 \quad // \text{mini-batch variance}$$

$$\hat{x}_i \leftarrow \frac{x_i - \mu_{\mathcal{B}}}{\sqrt{\sigma_{\mathcal{B}}^2 + \epsilon}} \quad // \text{normalize}$$

$$y_i \leftarrow \gamma \hat{x}_i + \beta \equiv \text{BN}_{\gamma, \beta}(x_i) \quad // \text{scale and shift}$$

# Batch Renormalization

- Issues with batch normalization
  - Different operations during training and testing
  - If small batch size then large changes between batches
- Batch renormalization
  - Start with batch norm
  - Start accumulating running averages for the mean and variance
  - Then gradually transition from using the per sample mean and variance to the running average mean and variance

**Input:** Values of  $x$  over a training mini-batch  $\mathcal{B} = \{x_{1\dots m}\}$ ; parameters  $\gamma, \beta$ ; current moving mean  $\mu$  and standard deviation  $\sigma$ ; moving average update rate  $\alpha$ ; maximum allowed correction  $r_{\max}, d_{\max}$ .

**Output:**  $\{y_i = \text{BatchRenorm}(x_i)\}$ ; updated  $\mu, \sigma$ .

$$\begin{aligned}\mu_{\mathcal{B}} &\leftarrow \frac{1}{m} \sum_{i=1}^m x_i \\ \sigma_{\mathcal{B}} &\leftarrow \sqrt{\epsilon + \frac{1}{m} \sum_{i=1}^m (x_i - \mu_{\mathcal{B}})^2} \\ r &\leftarrow \text{stop\_gradient} \left( \text{clip}_{[1/r_{\max}, r_{\max}]} \left( \frac{\sigma_{\mathcal{B}}}{\sigma} \right) \right) \\ d &\leftarrow \text{stop\_gradient} \left( \text{clip}_{[-d_{\max}, d_{\max}]} \left( \frac{\mu_{\mathcal{B}} - \mu}{\sigma} \right) \right) \\ \hat{x}_i &\leftarrow \frac{x_i - \mu_{\mathcal{B}}}{\sigma_{\mathcal{B}}} \cdot r + d \\ y_i &\leftarrow \gamma \hat{x}_i + \beta \\ \\ \mu &:= \mu + \alpha(\mu_{\mathcal{B}} - \mu) \quad // \text{Update moving averages} \\ \sigma &:= \sigma + \alpha(\sigma_{\mathcal{B}} - \sigma)\end{aligned}$$


---

**Inference:**  $y \leftarrow \gamma \cdot \frac{x - \mu}{\sigma} + \beta$

# Group Normalization

- Issues with batch normalization
  - Different operations during training and testing
  - If small batch size then large changes between batches
- Group normalization
  - Divide channels into groups
  - Compute mean and variance based on groups of channels

---

```
def GroupNorm(x, gamma, beta, G, eps=1e-5):
    # x: input features with shape [N,C,H,W]
    # gamma, beta: scale and offset, with shape [1,C,1,1]
    # G: number of groups for GN

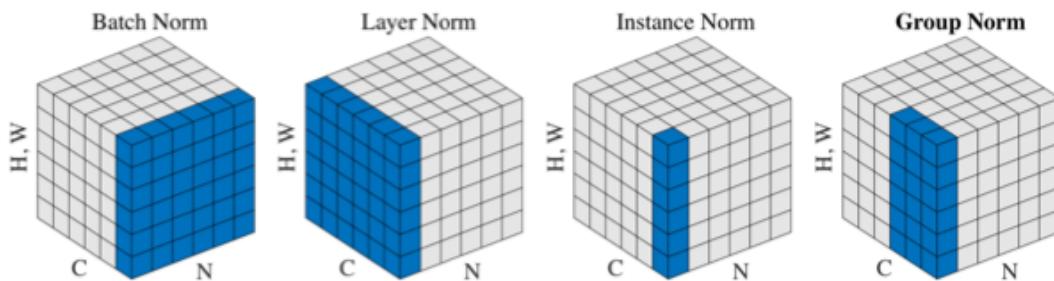
    N, C, H, W = x.shape
    x = tf.reshape(x, [N, G, C // G, H, W])

    mean, var = tf.nn.moments(x, [2, 3, 4], keep_dims=True)
    x = (x - mean) / tf.sqrt(var + eps)

    x = tf.reshape(x, [N, C, H, W])

    return x * gamma + beta
```

---



C = channel dimension  
 N = batch dimension  
 H = feature map height  
 W = feature map width

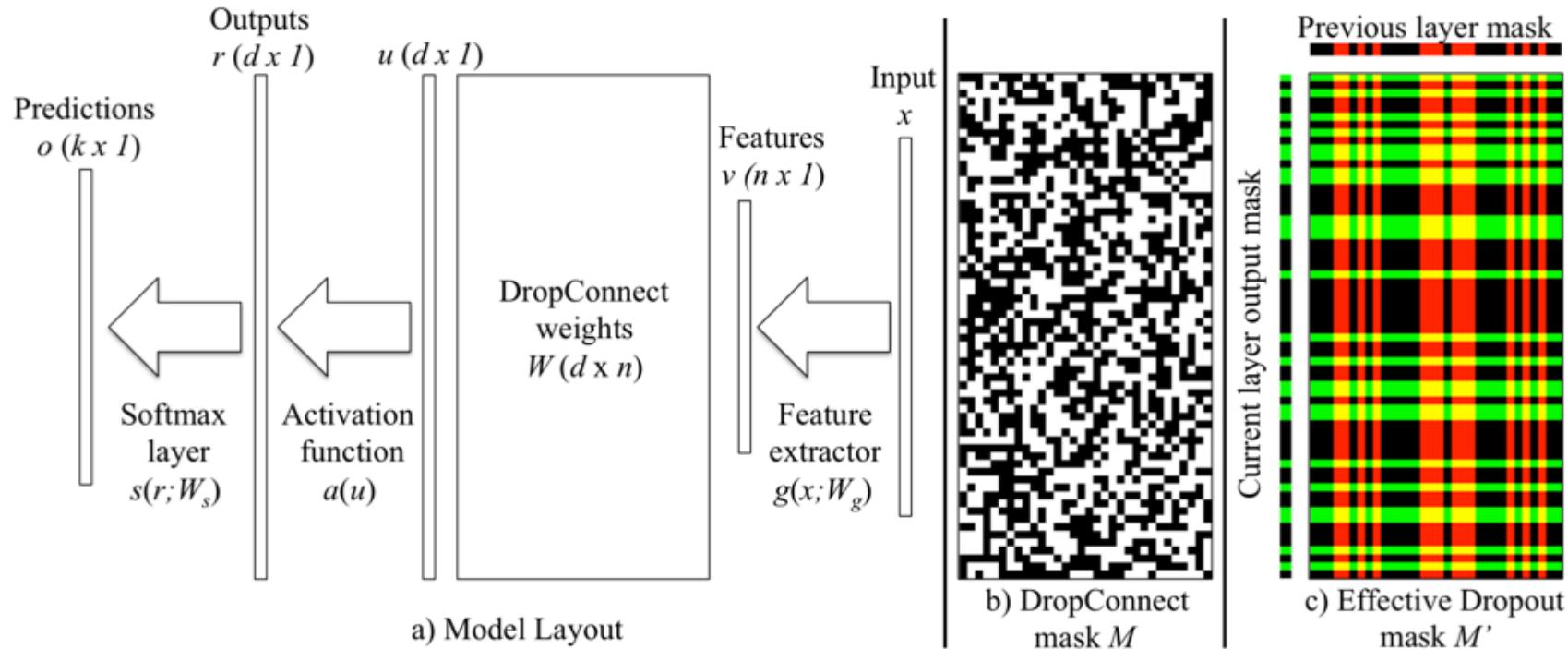
# Regularization

- It's possible to modify the forward path to help with regularization
- Example network modifications to improve regularization
  - Stochastic width
  - Stochastic depth
  - Noise addition in the network

# Stochastic Width (Dropout, DropConnect)

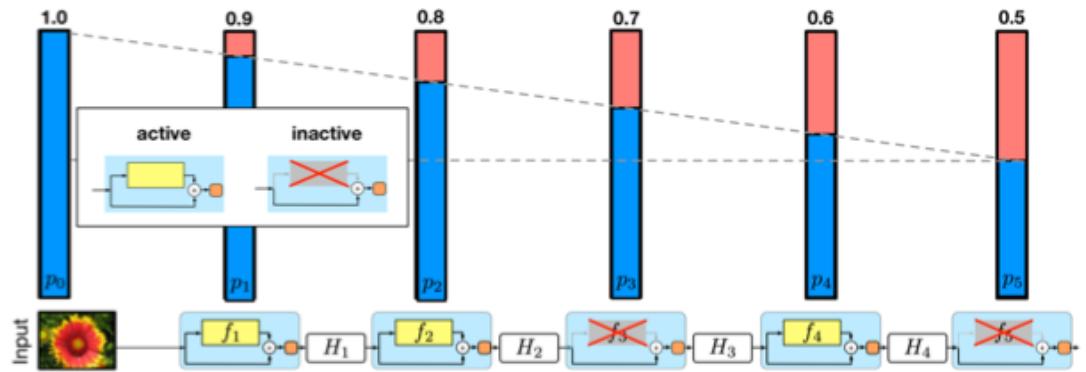
- The ideas behind stochastic width were most helpful in improving training with (multiple) large fully connected layers in earlier CNN designs
  - For wide networks this may be desirable
  - For narrow networks where the number of classes is on the order of or greater than the number of features this may be undesirable
  - Common current designs with global average pool and a single relatively smaller fully connected layer typically don't need to use stochastic width; but regardless, it's still a useful technique to know
- Dropout
  - Dropout zeros out a random set of layer outputs per batch
  - Implicitly it forces multiple groups of output features to be able to estimate a class
- DropConnect
  - DropConnect zeros out a random set of layer weights per batch
  - Implicitly it forces multiple groups of input features to be able to generate and output feature

# Stochastic Width (Dropout, DropConnect)



# Stochastic Depth (Layer Skipping)

- Stochastic depth (layer / building block skipping)
  - Only really used in very very deep residual networks
  - Implicitly it forces layers to do iterative refinement
- Notes
  - Probability of a layer being on or skipped (identity) is recommended to be layer dependent
  - Earlier in the network a layer is more likely to be on
  - Later in the network a layer is more likely to be bypassed
  - In testing a network output is scaled based on the probability that it was on during training



Note that  $H_n$  refers to the feature map at the output of operation  $n$ , not the layer itself

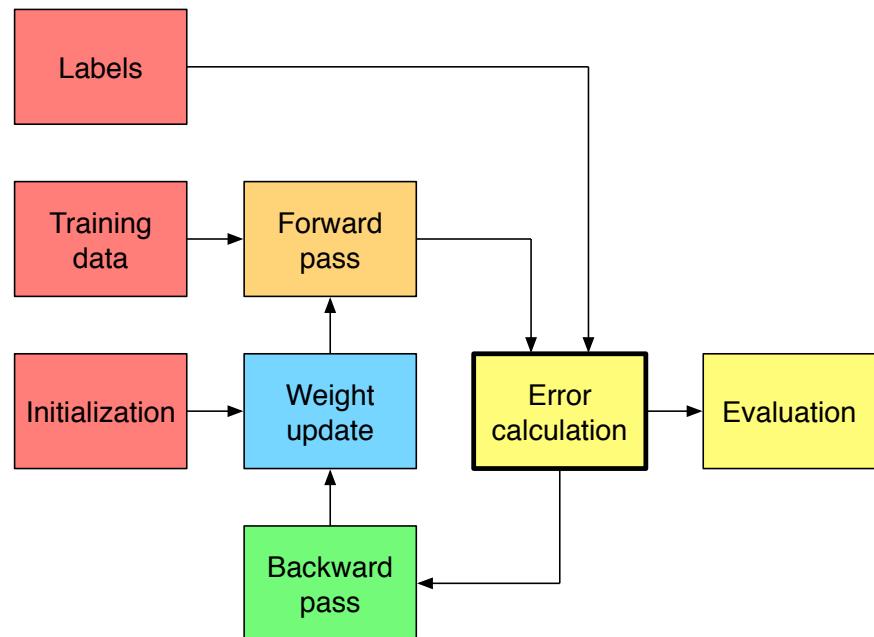
# Noise Addition

- Noise addition in the network
  - Feature maps
  - ReLU 0 point
  - ...
- Examples
  - Estimating or propagating gradients through stochastic neurons
    - <https://arxiv.org/abs/1305.2982>
  - Noisy activation functions
    - <https://arxiv.org/abs/1603.00391>
  - Dataset augmentation in feature space
    - <https://arxiv.org/abs/1702.05538>

# Error Calculation

# CNN Training Vs Function Optimization

- In the case of classification
  - Training with 1 loss (e.g., soft max – cross entropy)
  - Testing with a different loss (e.g., arg max)

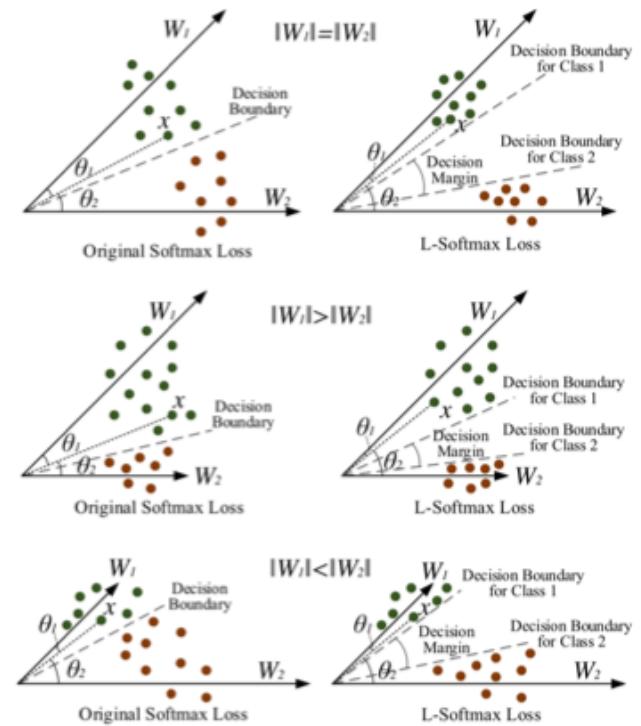


# 2 Broad Categories Of Loss Functions

- Classification
  - Prediction in a finite series of classes
  - Typically ...
    - Easier than regression
    - Complexity increases with number of classes
    - Complexity increases with similarity of classes
- Regression
  - Prediction in a continuum of values
  - Typically ...
    - More difficult than classification
    - Complexity increases with range and required resolution

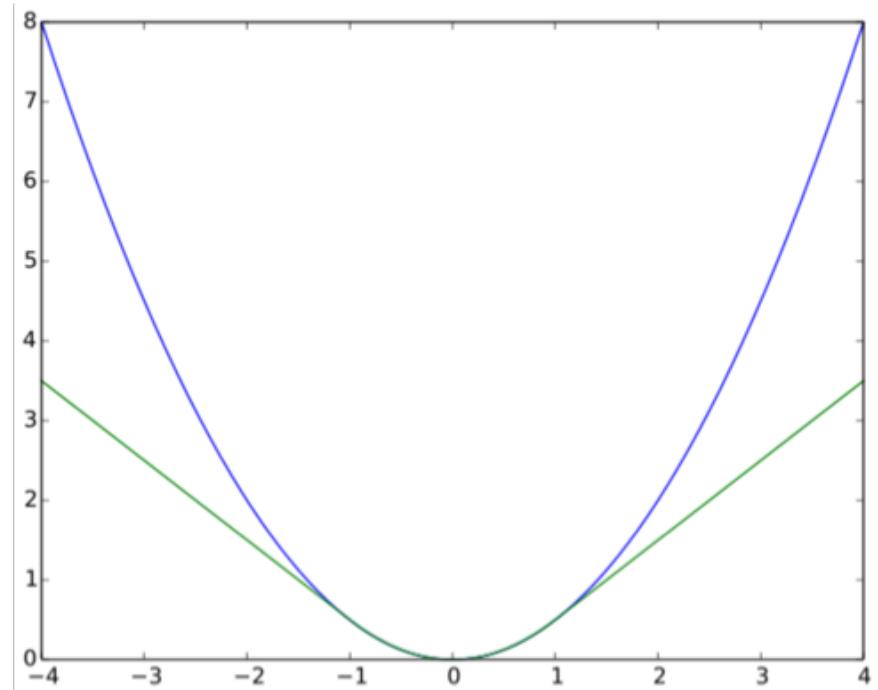
# Classification Loss

- Distinct outputs (classes)
- Softmax cross entropy loss function
  - Soft max effectively converts network outputs to a probability mass function
  - KL divergence for comparing 2 probability mass functions: target and network output
  - For a 1 hot target probability mass function KL divergence reduces to cross entropy
  - The calculus lecture notes derived a nice form for the gradient of the error at the output of soft max cross entropy with the input feature map to soft max
- Other options are possible
  - KL divergence with label smoothing, noise or overconfidence penalization
  - Large margin softmax
  - Optimal transport
  - ...



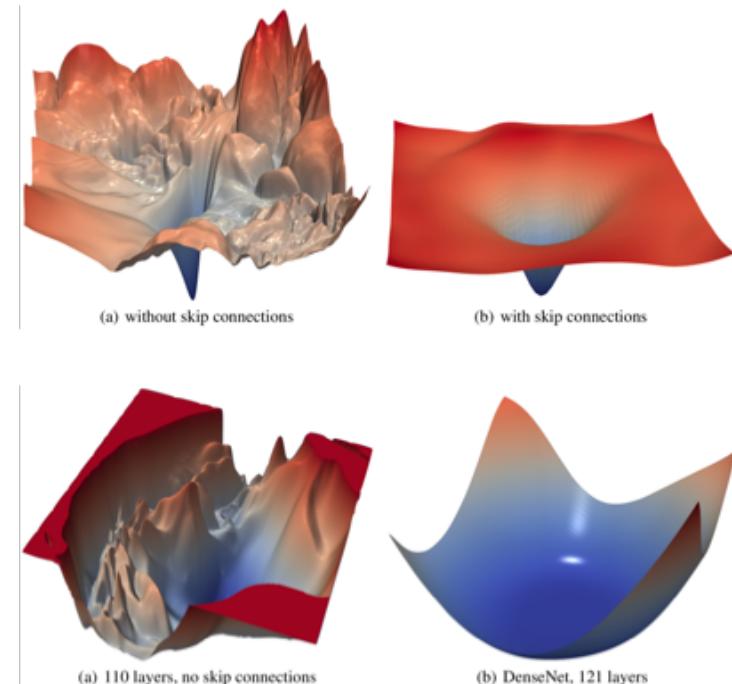
# Regression Loss

- Continuous valued output
  - Strategy: if you can quantize the continuous range and use classification instead of regression it may be better
- Standard  $l_p$  norms
  - $p = 1$
  - $p = 2$
- Other options are possible
  - Huber loss / smooth L1 loss (like  $l_2$  for small values and  $l_1$  for large values)



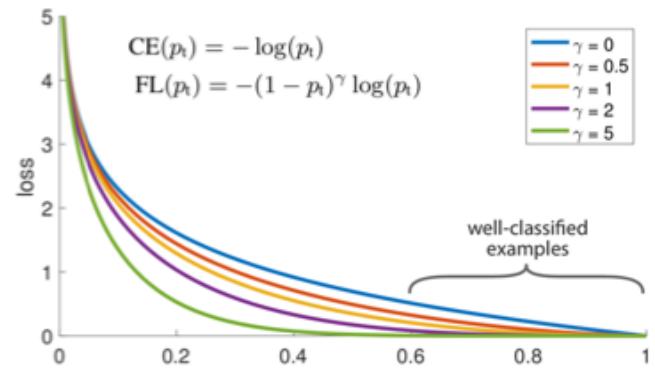
# Loss Surface Shapes

- The shape is a consequence of the choice of the data, network design and loss function
  - The weight update is going to attempt to find the lowest value of the function (and assume it also corresponds to the optimal value on the testing data)
  - Unfortunately, the loss surface is not convex
- You can't visualize it
  - You can think of shapes in  $\sim 1 - 4$  dimensions
  - The error (loss) is a function of the number of parameters (easily millions)
  - You can't (easily) think of shapes in millions dimensions
- But it has some characteristics that allow training to work
- Reminder: tell story on how to escape from jail



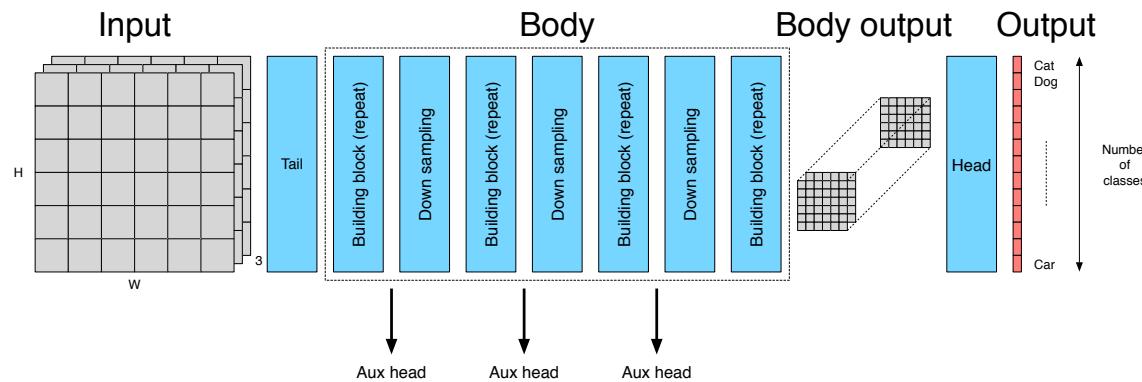
# Unequal Class Weightings

- Some classes are more difficult than others
- But so far the error calculation has treated all classes the same
- Strategy for modifications to the equal output class weighting of errors
  - Weight classes that are difficult (likely under represented in the training data) for the network more in the error computation
- Focal loss for dense object detection
  - <https://arxiv.org/abs/1708.02002>
  - Modifies cross entropy based on the inverse of category likelihood and probability when misclassified



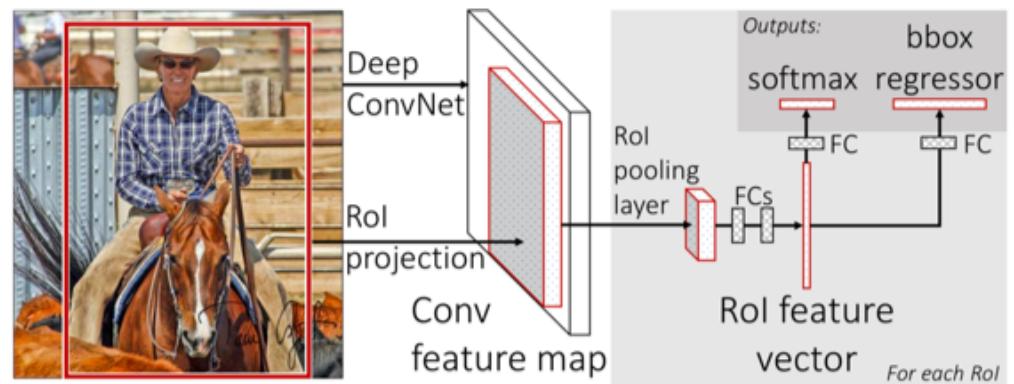
# Auxiliary Network Heads

- Features strong but poorly localized at the output of the body
  - Features are better localized but weaker earlier on in the network
  - While weaker, they're potentially still strong enough to predict classes, just not as accurately
- Idea: use auxiliary network heads during training to provide gradient information directly into the middle of the network
- Note: has possible drawback of getting the parameters stuck too much at a local minima



# Multiple Network Heads

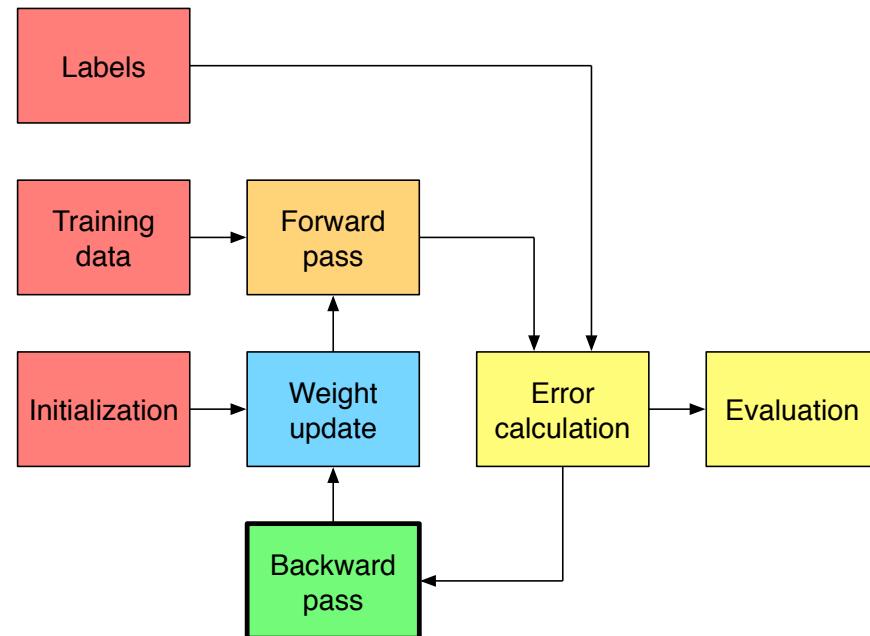
- Sometimes a network tail and body have multiple heads, each that accomplishes a different task
  - Want to optimize the performance of the full network
  - So need to create a loss that's combines the losses of all the heads
  - Multi task / combined function
- It's common to do this in multiple object detection networks
  - Classification of boxes as bounding objects and dimension modifications
  - Classification of objects in the bounding boxes



# Backward Pass

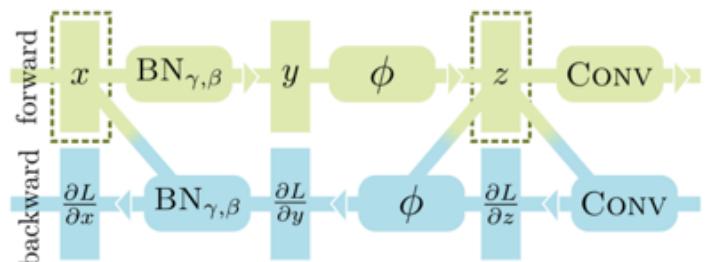
# Running Out Of Memory Is No Fun

- Reverse mode automatic differentiation
  - Covered in the calculus lecture
  - Basically stays the same
- But possibly make a modifications to address a practical issue: memory (or a lack thereof)
- Situation
  - Typically want larger batch sizes
  - This increases memory
  - Note that gradient computations in the backward pass are dependent on feature maps in the forward pass
  - End up running out of memory
  - Also, moving memory around is typically less efficient than computing

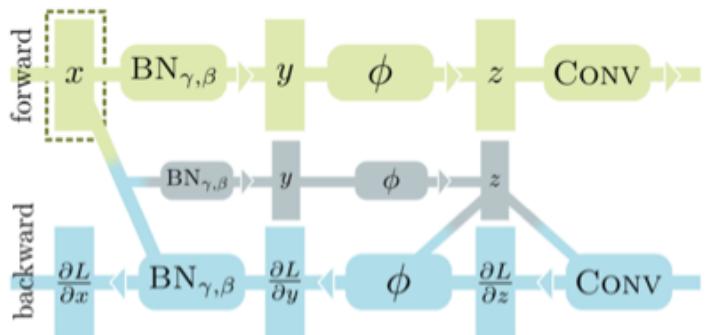


# Checkpointing

- A strategy for addressing running out of memory
  - Trade increased computation for reduced memory
  - A collection of techniques that falls under the umbrella of checkpointing
  - Also, change some non invertible operations in the forward pass to similar but invertible versions and use these in a similar way
- The data-flow equations of checkpointing in reverse automatic differentiation
  - <https://www-sop.inria.fr/tropics/papers/DauvergneHascoet06.pdf>
- Training deep nets with sublinear memory cost
  - <https://arxiv.org/pdf/1604.06174.pdf>
- Memory-efficient backpropagation through time
  - <https://arxiv.org/abs/1606.03401>
- For a nice implementation of this and figures see  
<https://github.com/openai/gradient-checkpointing>



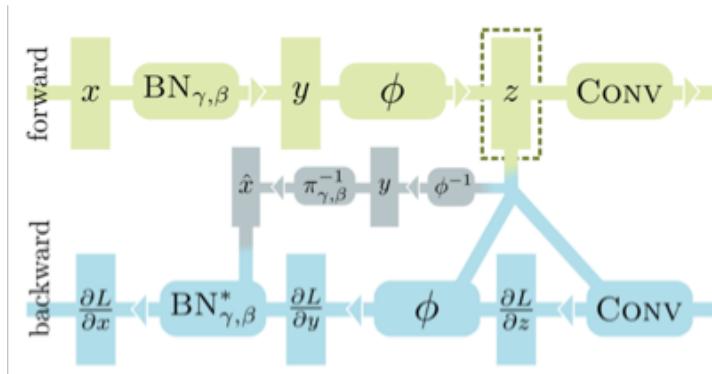
(a) Standard building block (memory-inefficient)



(b) Checkpointing [4, 21]

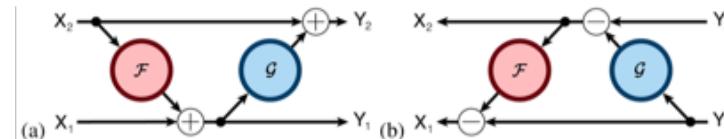
# In Place Activated Batch Norm

- Strategy
  - Replaces batch norm  $\rightarrow$  activation with a single layer and uses leaky ReLU vs ReLU to allow inversion through the nonlinearity to save  $\sim$  50% of memory
  - Remember the word “bijection” from the discussion of functions
- In-place activated batchnorm for memory-optimized training of DNNs
  - <https://arxiv.org/abs/1712.02616>
  - See also: <https://blog.mapillary.com/update/2017/12/08/massive-memory-savings-for-training-modern-deep-learning-architectures.html>



# Reversible Architectures

- Strategy
  - In place activated batch norm made the pointwise nonlinearity invertible
  - Question: is it possible to make the whole network (or at least large blocks of it) invertible
- RevNet
  - Apologies: I know you thought you were done learning new xNet names
  - Defines a different residual network such that each layers output can be derived from the previous layers output
  - The reversible residual network: backpropagation without storing activations
    - <https://arxiv.org/pdf/1707.04585.pdf>
- Perhaps less popular to do this in practice, but it's worth being aware of as a generally useful idea

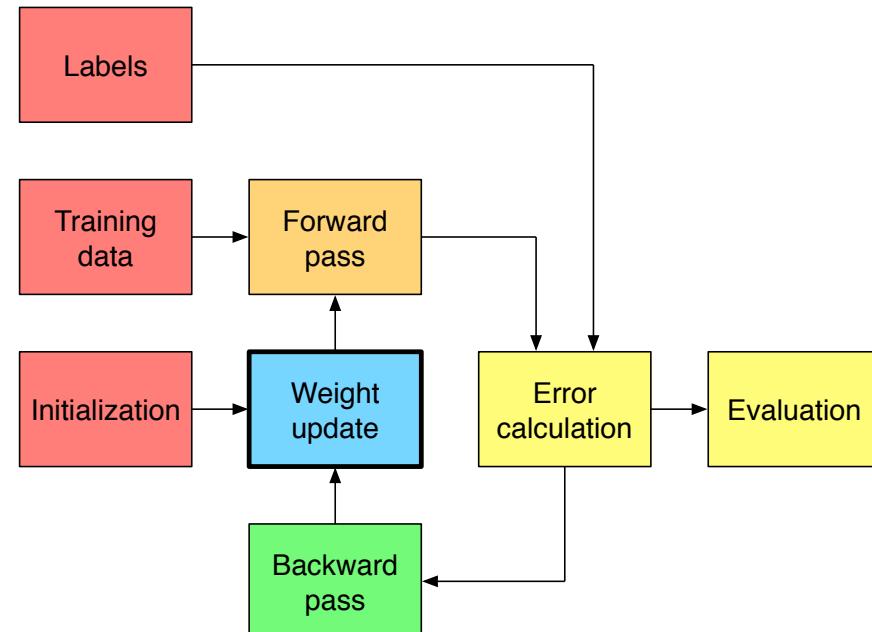


Technique	Spatial Complexity (Activations)	Computational Complexity
Naive	$\mathcal{O}(L)$	$\mathcal{O}(L)$
Checkpointing [20]	$\mathcal{O}(\sqrt{L})$	$\mathcal{O}(L)$
Recursive Checkpointing [5]	$\mathcal{O}(\log L)$	$\mathcal{O}(L \log L)$
Reversible Networks (Ours)	$\mathcal{O}(1)$	$\mathcal{O}(L)$

# Weight Update

# CNN Training Vs Function Optimization

- Classic gradient descent
  - Runs through all data samples
  - Then makes an update
- Modifications to classical gradient descent considered in this section serve at least 1 of 3 purposes
  - Improve accuracy (convergence)
  - Improve generalization (regularization)
  - Improve performance (speed)

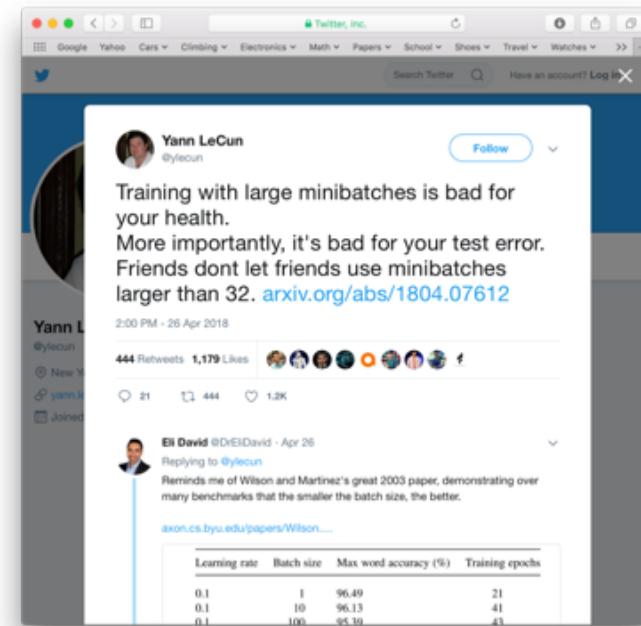


# Convergence

- Items described here for improving convergence include
  - Batch size
  - Gradient update method
  - Parameter update schedule

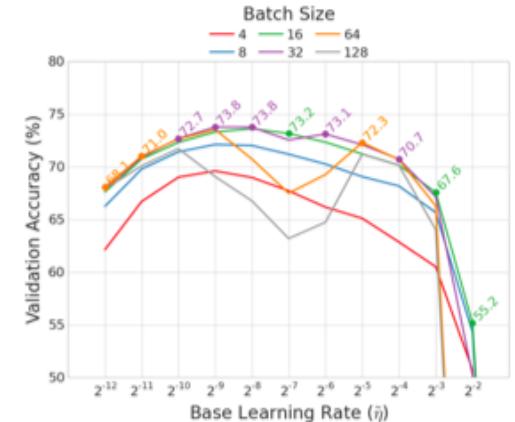
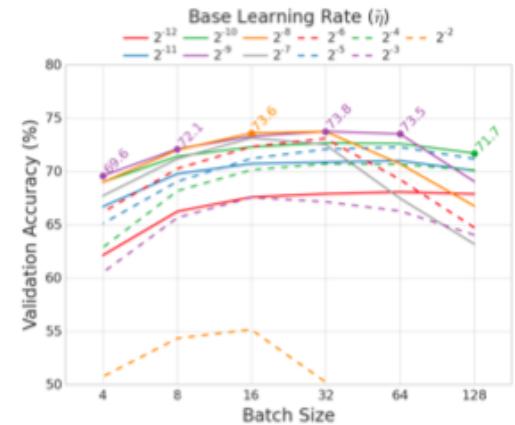
# Batch Size

- Some notational things, just be aware of
  - 1 input, 1 update (stochastic gradient descent)
  - Batch of inputs, 1 update(mini batch stochastic gradient descent)
  - All inputs, 1 update (gradient descent)
- What does the choice of batch size affect?
  - Memory (smaller == less)
  - Serial updates (larger == faster, to a saturation lim)
  - Parallel updates (larger == faster, more machines)
  - Gradient noise (larger == less)
  - Batch norm effectiveness(larger == better)
  - Accuracy on training data (maybe smaller == better)
  - Accuracy on testing data (maybe smaller == better)

Figure from <https://twitter.com/ylecun/status/989610208497360896?lang=en>

# Batch Size For A Single Machine

- How to select the batch size for a single machine
  - Not a horrible starting point: 32
  - Other not horrible strategy: increase size until the training GPU runs out of memory and use that, unless it's too small and then do some aggregation
- Notes
  - Train longer, generalize better: closing the generalization gap in large batch training of neural networks
    - <https://arxiv.org/abs/1705.08741>
  - Revisiting small batch training for deep neural networks
    - <https://arxiv.org/abs/1804.07612>
  - Other
    - <https://machinelearningmastery.com/gentle-introduction-mini-batch-gradient-descent-configure-batch-size/>
    - <https://stats.stackexchange.com/questions/140811/how-large-should-the-batch-size-be-for-stochastic-gradient-descent>



# Weight Update Considerations

- Notation
  - Weights  $\mathbf{w}$
  - Error  $e(\mathbf{w})$
  - Gradient  $\mathbf{g}, g_i = \partial e / \partial w_i$
  - Hessian  $\mathbf{H}, H_{i,j} = \partial^2 e / \partial w_i \partial w_j$
- 2nd order approximation of the error about a point  $\mathbf{w}_0$ 
  - Error = current error + 1st order approximation of change + 2nd order correction
  - $$e(\mathbf{w}) \approx e(\mathbf{w}_0) + (\mathbf{w} - \mathbf{w}_0)^T \mathbf{g} + 0.5 (\mathbf{w} - \mathbf{w}_0)^T \mathbf{H} (\mathbf{w} - \mathbf{w}_0)$$
- 2nd order Newton's method (reminder: show quick derivation)
  - $\mathbf{H} > 0$  (positive definite)
  - $\mathbf{w} \leftarrow \mathbf{w} - \mathbf{H}^{-1} \mathbf{g}$

# Weight Update Considerations

- 1st order gradient descent
  - $\mathbf{w}_{t+1} = \mathbf{w}_t - \alpha \mathbf{g}$
  - $e(\mathbf{w}_t - \alpha \mathbf{g}) \approx \begin{array}{lll} e(\mathbf{w}_t) & -\alpha \mathbf{g}^T \mathbf{g} & + 0.5 \alpha^2 \mathbf{g}^T \mathbf{H} \mathbf{g} \\ \text{Orig} & \text{Improvement} & \text{2nd order correction} \end{array}$
- When the 2nd order correction is positive the optimal step size is (show derivation)
  - $\alpha = (\mathbf{g}^T \mathbf{g}) / (\mathbf{g}^T \mathbf{H} \mathbf{g})$
- Pertinent note: gradient descent doesn't exploit curvature as captured in the  $\mathbf{H}$  matrix, but different directions have different shapes
- Random note: we also haven't discussed persistent excitation (is the system input / output identifiable?)

# Weight Update Notes

- Weight update methods need to deal with non convex error surfaces with 3 types of critical points
  - Minima
  - Maxima
  - Saddle (some directions minima, some maxima)
- Saddle points are the most common type of point in high dimensions
  - Argument: Imagine that minima and maxima are equally likely
  - A critical point requires 1000s to millions of derivatives all to be 0
  - Many more are a blend of positive and negative vs all positive or all negative
- Saddle points tend to have a moderately high error
  - Newton's method is attracted to critical points, critical points tend to be saddle points and saddle points tend to have moderately high error (1 reason why Newton's method is not commonly used for training CNNs)
  - Gradient descent methods aren't attracted specifically to saddle points and seem to be able to escape them (1 reason why they're used for training CNNs)

# Weight Update Notes

- Some error surface shapes that are tricky for gradient descent methods
  - Wide flat regions: tend to be tough to get through as the gradient is close to 0; sometimes momentum helps
  - Cliffs: unstable at the edge as gradients can become very large; sometimes gradient clipping helps
- A caution when optimizing a system with repeated transformations (like in a RNN)
  - Transformations scales gradients
  - If a transformation is repeatedly applied (as in a RNN) then it scales gradients repeatedly
  - If the scaling is large this causes gradient explosion, if the scaling is small this causes gradient vanishing
  - So ideally want the scale of a transformation that's applied many times to be close to 1
- Everything we've talked about only makes local updates
  - Note that gradient descent moves locally, usually just a small amount
  - Problem: if the region where the error is small is not near the current point
  - Hints at the importance of initialization and / or being able to make bigger jumps

# Weight Update Methods (Optimizers, Solvers)

- Algorithms without adaptive gradients
  - Stochastic gradient descent (SGD)
  - Stochastic gradient descent with momentum
    - Heavy ball (HB)
    - Nesterov accelerated gradient (NAG)
- Algorithms with adaptive gradients
  - AdaGrad
  - RMSProp
  - Adam
- Presentation styles
  - Deep Learning Book (chapter 8)
    - <https://www.deeplearningbook.org/contents/optimization.html>
  - The marginal value of adaptive gradient methods in machine learning
    - <https://arxiv.org/abs/1705.08292>

	SGD	HB	NAG	AdaGrad	RMSProp	Adam
$G_k$	I	I	I	$G_{k-1} + D_k$	$\beta_2 G_{k-1} + (1 - \beta_2) D_k$	$\frac{\beta_2}{1 - \beta_2^k} G_{k-1} + \frac{(1 - \beta_2)}{1 - \beta_2^k} D_k$
$\alpha_k$	$\alpha$	$\alpha$	$\alpha$	$\alpha$	$\alpha$	$\alpha \frac{1 - \beta_1}{1 - \beta_1^k}$
$\beta_k$	0	$\beta$	$\beta$	0	0	$\frac{\beta_1(1 - \beta_1^{k-1})}{1 - \beta_1^k}$
$\gamma$	0	0	$\beta$	0	0	0

**Table 1:** Parameter settings of algorithms used in deep learning. Here,  $D_k = \text{diag}(g_k \circ g_k)$  and  $G_k := H_k \circ H_k$ . We omit the additional  $\epsilon$  added to the adaptive methods, which is only needed to ensure non-singularity of the matrices  $H_k$ .

General algorithm form without adaptive gradient

$$w_{k+1} = w_k - \alpha_k \tilde{\nabla} f(w_k + \gamma_k(w_k - w_{k-1})) + \beta_k(w_k - w_{k-1})$$

General algorithm form with adaptive gradient

$$w_{k+1} = w_k - \alpha_k H_k^{-1} \tilde{\nabla} f(w_k + \gamma_k(w_k - w_{k-1})) + \beta_k H_k^{-1} H_{k-1}(w_k - w_{k-1})$$

$$H_k = \text{diag} \left( \left\{ \sum_{i=1}^k \eta_i g_i \circ g_i \right\}^{1/2} \right)$$

# Stochastic Gradient Descent

- Stochastic gradient descent
  - Too much data to use gradient descent so use batches
- From the calculus lectures
  - Starting from the gradient of the error with respect to the filter parameters
  - The gradient points in the direction of the local maximum change of the error with respect to the filter parameters
  - To reduce the error take a step in the opposite (negative) direction
- Similar to Hebbian theory in biology
  - Neurons that fire together wire together
  - This adjusts up the neurons that work together more

---

**Algorithm 8.1** Stochastic gradient descent (SGD) update at training iteration  $k$ 

**Require:** Learning rate  $\epsilon_k$ .

**Require:** Initial parameter  $\theta$

**while** stopping criterion not met **do**

    Sample a minibatch of  $m$  examples from the training set  $\{\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(m)}\}$  with corresponding targets  $\mathbf{y}^{(i)}$ .

    Compute gradient estimate:  $\hat{\mathbf{g}} \leftarrow +\frac{1}{m} \nabla_{\theta} \sum_i L(f(\mathbf{x}^{(i)}; \theta), \mathbf{y}^{(i)})$

    Apply update:  $\theta \leftarrow \theta - \epsilon \hat{\mathbf{g}}$

**end while**

---

## Hyper parameters that require a choice

- Initialization (previously discussed)
- Batch size (previously discussed)
- Batch selection (previously discussed)
- Step size (will discuss next)
- Stopping criteria (will discuss soon)

# Stochastic Gradient Descent With Momentum

- Momentum adds short term memory to the update (heavy ball or Nesterov)
- Comments
  - Accumulates an exponentially decaying moving average of past gradients
  - Improves poor conditioning of the Hessian and variance in the stochastic gradient
  - Moves are now in the direction of gradient + momentum
- Paper and nice discussion
  - Why momentum really works (note: excellent post)
    - <https://distill.pub/2017/momentum/>
  - On the importance of initialization and momentum in deep learning
    - <http://proceedings.mlr.press/v28/sutskever13.pdf>

---

**Algorithm 8.2** Stochastic gradient descent (SGD) with momentum

---

**Require:** Learning rate  $\epsilon$ , momentum parameter  $\alpha$ .

**Require:** Initial parameter  $\theta$ , initial velocity  $v$ .

**while** stopping criterion not met **do**

    Sample a minibatch of  $m$  examples from the training set  $\{\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(m)}\}$  with corresponding targets  $\mathbf{y}^{(i)}$ .

    Compute gradient estimate:  $\mathbf{g} \leftarrow \frac{1}{m} \nabla_{\theta} \sum_i L(f(\mathbf{x}^{(i)}; \theta), \mathbf{y}^{(i)})$

    Compute velocity update:  $\mathbf{v} \leftarrow \alpha \mathbf{v} - \epsilon \mathbf{g}$

    Apply update:  $\theta \leftarrow \theta + \mathbf{v}$

**end while**

---

**Algorithm 8.3** Stochastic gradient descent (SGD) with Nesterov momentum

---

**Require:** Learning rate  $\epsilon$ , momentum parameter  $\alpha$ .

**Require:** Initial parameter  $\theta$ , initial velocity  $v$ .

**while** stopping criterion not met **do**

    Sample a minibatch of  $m$  examples from the training set  $\{\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(m)}\}$  with corresponding labels  $\mathbf{y}^{(i)}$ .

    Apply interim update:  $\tilde{\theta} \leftarrow \theta + \alpha v$

    Compute gradient (at interim point):  $\mathbf{g} \leftarrow \frac{1}{m} \nabla_{\tilde{\theta}} \sum_i L(f(\mathbf{x}^{(i)}; \tilde{\theta}), \mathbf{y}^{(i)})$

    Compute velocity update:  $\mathbf{v} \leftarrow \alpha \mathbf{v} - \epsilon \mathbf{g}$

    Apply update:  $\theta \leftarrow \theta + \mathbf{v}$

**end while**

---

# AdaGrad

- Inversely scales individual elements of the gradient based on the square root of the square of all previous updates
  - Parameters with large updates have learning rates that are reduced a lot
  - Parameters with small updates have learning rates that are reduced a little (allowing relatively more progress in areas with small gradients)
  - May choose to start this after the initial updates have stabilized
  - Works well with sparse gradients
- Adaptive subgradient methods for online learning and stochastic optimization
  - <http://www.jmlr.org/papers/volume12/duchi11a/duchi11a.pdf>

---

**Algorithm 8.4** The AdaGrad algorithm
 

---

**Require:** Global learning rate  $\epsilon$

**Require:** Initial parameter  $\theta$

**Require:** Small constant  $\delta$ , perhaps  $10^{-7}$ , for numerical stability

Initialize gradient accumulation variable  $r = \mathbf{0}$

**while** stopping criterion not met **do**

  Sample a minibatch of  $m$  examples from the training set  $\{\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(m)}\}$  with corresponding targets  $\mathbf{y}^{(i)}$ .

  Compute gradient:  $\mathbf{g} \leftarrow \frac{1}{m} \nabla_{\theta} \sum_i L(f(\mathbf{x}^{(i)}; \theta), \mathbf{y}^{(i)})$

  Accumulate squared gradient:  $\mathbf{r} \leftarrow \mathbf{r} + \mathbf{g} \odot \mathbf{g}$

  Compute update:  $\Delta\theta \leftarrow -\frac{\epsilon}{\delta + \sqrt{\mathbf{r}}} \odot \mathbf{g}$ . (Division and square root applied element-wise)

  Apply update:  $\theta \leftarrow \theta + \Delta\theta$

**end while**

---

# RMSProp

- Like AdaGrad but with an exponentially weighted forgetting factor on the gradient scale
  - Gets around some of the initial variance of the gradient scale problems that AdaGrad has
  - Exponential forgetting gives it a bit more of a local flavor which seems right
  - Works well with sparse gradients and non stationarity
- Neural networks for machine learning
  - [http://www.cs.toronto.edu/%7Etijmen/csc321/slides/lecture\\_slides\\_lec6.pdf](http://www.cs.toronto.edu/%7Etijmen/csc321/slides/lecture_slides_lec6.pdf)

---

**Algorithm 8.5** The RMSProp algorithm
 

---

**Require:** Global learning rate  $\epsilon$ , decay rate  $\rho$ .

**Require:** Initial parameter  $\theta$

**Require:** Small constant  $\delta$ , usually  $10^{-6}$ , used to stabilize division by small numbers.

Initialize accumulation variables  $r = 0$

**while** stopping criterion not met **do**

    Sample a minibatch of  $m$  examples from the training set  $\{\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(m)}\}$  with corresponding targets  $\mathbf{y}^{(i)}$ .

    Compute gradient:  $\mathbf{g} \leftarrow \frac{1}{m} \nabla_{\theta} \sum_i L(f(\mathbf{x}^{(i)}; \theta), \mathbf{y}^{(i)})$

    Accumulate squared gradient:  $\mathbf{r} \leftarrow \rho \mathbf{r} + (1 - \rho) \mathbf{g} \odot \mathbf{g}$

    Compute parameter update:  $\Delta\theta = -\frac{\epsilon}{\sqrt{\delta+r}} \odot \mathbf{g}$ . ( $\frac{1}{\sqrt{\delta+r}}$  applied element-wise)

    Apply update:  $\theta \leftarrow \theta + \Delta\theta$

**end while**

---

# RMSProp With Momentum

- Add Nesterov momentum to RMSProp
- Why did I include this beyond the fact that it works in some cases?
  - SGD started us down a path with a nice intuition
  - We added momentum to that which has some plausibility (new direction = old direction + correction)
  - AdaGrad starts to feel like we're playing some games with heuristics, though motivated by intuition of looking at many results
  - RMSProp feels this way even more as it's a modification to AdaGrad
  - By the time we get to RMSProp with momentum we start to think of both creating modifications around gradient descent and combining different modifications that seem to work well together
  - This combination of different ideas is mentally setting us up for learning solvers in a few slides

---

**Algorithm 8.6** RMSProp algorithm with Nesterov momentum
 

---

**Require:** Global learning rate  $\epsilon$ , decay rate  $\rho$ , momentum coefficient  $\alpha$ .  
**Require:** Initial parameter  $\theta$ , initial velocity  $v$ .

Initialize accumulation variable  $r = \mathbf{0}$

**while** stopping criterion not met **do**

    Sample a minibatch of  $m$  examples from the training set  $\{\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(m)}\}$  with corresponding targets  $\mathbf{y}^{(i)}$ .

    Compute interim update:  $\tilde{\theta} \leftarrow \theta + \alpha v$

    Compute gradient:  $\mathbf{g} \leftarrow \frac{1}{m} \nabla_{\tilde{\theta}} \sum_i L(f(\mathbf{x}^{(i)}; \tilde{\theta}), \mathbf{y}^{(i)})$

    Accumulate gradient:  $r \leftarrow \rho r + (1 - \rho) \mathbf{g} \odot \mathbf{g}$

    Compute velocity update:  $v \leftarrow \alpha v - \frac{\epsilon}{\sqrt{r}} \odot \mathbf{g}$ . ( $\frac{1}{\sqrt{r}}$  applied element-wise)

    Apply update:  $\theta \leftarrow \theta + v$

**end while**

---

# Adam

- Adaptive moments
- Comments
  - Exponential moving averages of the gradient (mean) and the squared gradient (variance)
  - Corrects for the bias in the 0 initialized estimates
  - Update is the direction of the gradient mean with individual elements scaled by the square root of the gradient variance
- Adam: a method for stochastic optimization
  - <https://arxiv.org/abs/1412.6980>

---

**Algorithm 8.7** The Adam algorithm
 

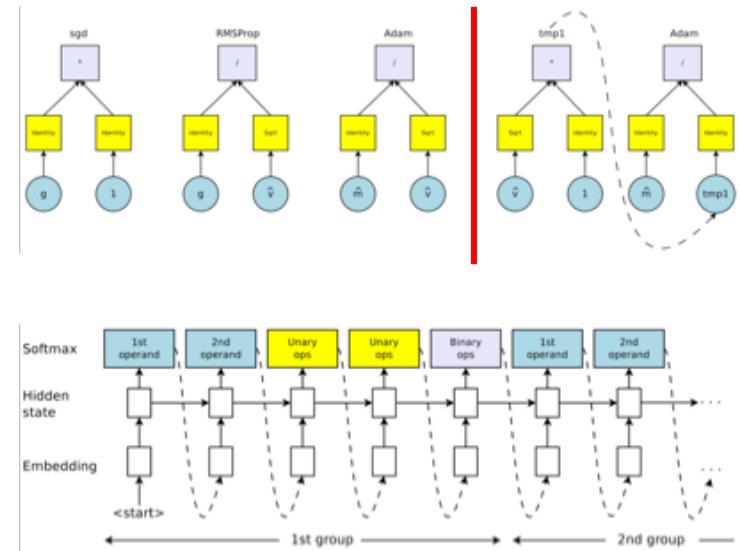
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**Require:** Step size  $\epsilon$  (Suggested default: 0.001)  
**Require:** Exponential decay rates for moment estimates,  $\rho_1$  and  $\rho_2$  in  $[0, 1]$ .  
 (Suggested defaults: 0.9 and 0.999 respectively)  
**Require:** Small constant  $\delta$  used for numerical stabilization. (Suggested default:  
 $10^{-8}$ )  
**Require:** Initial parameters  $\theta$   
 Initialize 1st and 2nd moment variables  $s = \mathbf{0}$ ,  $r = \mathbf{0}$   
 Initialize time step  $t = 0$   
**while** stopping criterion not met **do**  
 Sample a minibatch of  $m$  examples from the training set  $\{\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(m)}\}$  with  
 corresponding targets  $\mathbf{y}^{(i)}$ .  
 Compute gradient:  $\mathbf{g} \leftarrow \frac{1}{m} \nabla_{\theta} \sum_i L(f(\mathbf{x}^{(i)}; \theta), \mathbf{y}^{(i)})$   
 $t \leftarrow t + 1$   
 Update biased first moment estimate:  $\hat{s} \leftarrow \rho_1 s + (1 - \rho_1) \mathbf{g}$   
 Update biased second moment estimate:  $\hat{r} \leftarrow \rho_2 r + (1 - \rho_2) \mathbf{g} \odot \mathbf{g}$   
 Correct bias in first moment:  $\hat{s} \leftarrow \frac{\hat{s}}{1 - \rho_1^t}$   
 Correct bias in second moment:  $\hat{r} \leftarrow \frac{\hat{r}}{1 - \rho_2^t}$   
 Compute update:  $\Delta\theta = -\epsilon \frac{\hat{s}}{\sqrt{\hat{r} + \delta}}$  (operations applied element-wise)  
 Apply update:  $\theta \leftarrow \theta + \Delta\theta$   
**end while**


---

# Learning A New Solver

- Flashback to the design lecture
  - We spent a considerable amount of time discussing CNN designs created by humans
  - Then briefly spent time discussing that we could put various configurable network design building blocks in an optimizer and algorithmically design a network
  - We also did this for nonlinearities, using an optimizer to find a replacement for ReLU
- Now think about right now
  - We just spent a considerable amount of time discussing weight update methods created by humans
  - Guess what: we can put various configurable weight update building blocks in an optimizer and algorithmically find a solver (and also a learning rate schedule)
- Neural optimizer search with reinforcement learning
  - <https://arxiv.org/abs/1709.07417>



# Learning A New Solver

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  - <https://arxiv.org/abs/1709.07417>

**Operands:**  $g, g^2, g^3, \hat{m}, \hat{v}, \hat{\gamma}, \text{sign}(g), \text{sign}(\hat{m}), 1, 2, \epsilon \sim N(0, 0.01), 10^{-4}w, 10^{-3}w, 10^{-2}w, 10^{-1}w, \text{Adam and RMSProp.}$

**Unary functions** which map input  $x$  to:  $x, -x, e^x, \log|x|, \sqrt{|x|}, \text{clip}(x, 10^{-5}), \text{clip}(x, 10^{-4}), \text{clip}(x, 10^{-3}), \text{drop}(x, 0.1), \text{drop}(x, 0.3), \text{drop}(x, 0.5)$  and  $\text{sign}(x)$ .

**Binary functions** which map  $(x, y)$  to  $x + y$  (addition),  $x - y$  (subtraction),  $x * y$  (multiplication),  $\frac{x}{y+\delta}$  (division),  $x^y$  (exponentiation) or  $x$  (keep left).

linear decay:  $ld = 1 - \frac{t}{T}$ .

cyclical decay:  $cd_n = 0.5 * (1 + \cos(2\pi n \frac{t}{T}))$ .

restart decay:  $rd_n = 0.5 * (1 + \cos(\pi \frac{(tn)\%T}{T}))$  introduced in [Loshchilov & Hutter \(2017\)](#).

annealed noise:  $\epsilon_t \sim N(0, 1/(1+t)^{0.55})$  inspired by [Neelakantan et al. \(2016\)](#).

# Learning A New Solver

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  - We spent a considerable amount of time discussing CNN designs created by humans
  - Then briefly spent time discussing that we could put various configurable network design building blocks in an optimizer and algorithmically design a network
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- Now think about right now
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- Neural optimizer search with reinforcement learning
  - <https://arxiv.org/abs/1709.07417>

**PowerSign:**  $\alpha^{f(t)*\text{sign}(g)*\text{sign}(m)} * g$ . Some sampled update rules in this family include:

- $e^{\text{sign}(g)*\text{sign}(m)} * g$
- $e^{ld*\text{sign}(g)*\text{sign}(m)} * g$
- $e^{cd*\text{sign}(g)*\text{sign}(m)} * g$
- $2^{\text{sign}(g)*\text{sign}(m)} * g$

**AddSign:**  $(\alpha + f(t) * \text{sign}(g) * \text{sign}(m)) * g$ . Some sampled update rules in this family include:

- $(1 + \text{sign}(g) * \text{sign}(m)) * g$
  - $(1 + ld * \text{sign}(g) * \text{sign}(m)) * g$
  - $(1 + cd * \text{sign}(g) * \text{sign}(m)) * g$
  - $(2 + \text{sign}(g) * \text{sign}(m)) * g$
- 

$ld * cd$ , which we call *linear cosine decay*.

$(ld + \epsilon_t) * cd + 0.001$ , which we call *noisy linear decay*.

# Which Solver To Use?

- Think of the below suggestions as a starting point for an initial training when you're still sorting out variations in network design
- Suggestions
  - SGD with momentum
    - Maybe slower
    - Maybe generalizes better
  - Adam
    - Maybe faster
    - Maybe generalizes worse



# Learning Rate Update Schedules

- This is typically encoded as a hyper parameter
- Types
  - Fixed step schedule
  - Continual step schedule
  - Adaptive step schedule
  - Hyper gradient descent
- Online learning rate adaptation with hypergradient descent
  - <https://arxiv.org/abs/1703.04782>

# Regularization

- Example methods
  - Weight decay
  - Gradient noise
  - Gradient clipping

# Weight Decay – L2

- Basic idea
  - Large weights make overfitting more likely
  - Introduce a term in the error calculation to penalize large weights, acts as a regularizer to improve generalization
  - The effect of the introduction of this term in the error calculation is a decay of the weights during the weight update step (hence the name weight decay)
- 2 common penalty terms
  - L2 norm:  $e_{\text{decay}}(\mathbf{w}) = e_{\text{original}}(\mathbf{w}) + \lambda \sum_k (w^2(k))$
  - L1 norm:  $e_{\text{decay}}(\mathbf{w}) = e_{\text{original}}(\mathbf{w}) + \lambda \sum_k |w(k)|$
- The regularization strategy is also called ridge regression or Tikhonov regularization

# Weight Decay – L2

- Resulting weight update
  - L2 norm:  $\mathbf{w}_{\text{decay}} = \mathbf{w}_{\text{original}} - \alpha \frac{\partial e}{\partial \mathbf{w}} - \alpha \lambda \mathbf{w}$
  - L1 norm:  $\mathbf{w}_{\text{decay}} = \mathbf{w}_{\text{original}} - \alpha \frac{\partial e}{\partial \mathbf{w}} - \alpha \lambda \text{sign}(\mathbf{w})$
- Comments
  - L2 regularization is more common than L1 regularization
  - L1 regularization tends to promote more sparsity
  - It's common to only apply this to multiplicative weights and not additive weights (appropriate due to the scale of additive weights being a function of the feature map and multiplicative weight scales)
- A simple weight decay can improve generalization
  - <https://papers.nips.cc/paper/563-a-simple-weight-decay-can-improve-generalization.pdf>

# Gradient Noise

- Basic idea
  - Add noise to the gradient used by the weight update to improve regularization
- On the energy landscape of deep networks
  - <https://arxiv.org/abs/1511.06485>
  - Adds noise to the gradient via an annealing strategy to control the number of local minima in the error surface, starting from a simple shaped surface and transitioning to the original complex shaped surface
- For variations on this theme see
  - Adding gradient noise improves learning for very deep networks
    - <https://arxiv.org/abs/1511.06807>
  - The effects of adding noise during backpropagation training on a generalization performance
    - <https://ieeexplore.ieee.org/document/6796981>

# Gradient Clipping

- RNNs, as they use the same transform repeatedly, have a potential problem with exploding or vanishing gradients
  - Learning long-term dependencies with gradient descent is difficult
    - <http://www.iro.umontreal.ca/~lisa/poiteurs/ieeetrnn94.pdf>
- One method for addressing the exploding gradient problem is to use gradient clipping
  - If the magnitude of the gradient exceeds a threshold clip the magnitude to the threshold
  - On the difficulty of training Recurrent Neural Networks
    - <https://arxiv.org/abs/1211.5063>
- Note that this may introduce some subtle issues with respect to back prop

---

**Algorithm 1** Pseudo-code for norm clipping the gradients whenever they explode

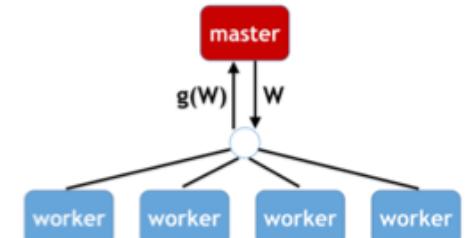
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```
 $\hat{g} \leftarrow \frac{\partial \mathcal{E}}{\partial \theta}$ 
if  $\|\hat{g}\| \geq \text{threshold}$  then
     $\hat{g} \leftarrow \frac{\text{threshold}}{\|\hat{g}\|} \hat{g}$ 
end if
```

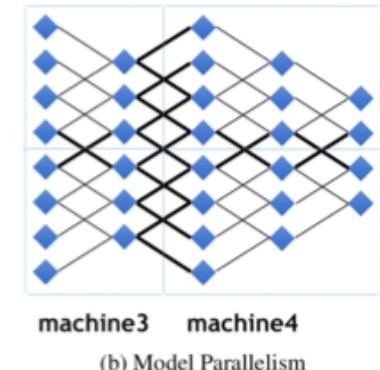
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# Parallelization

- Performance == training speed
  - Not accuracy, we'll call that accuracy
- Motivation
  - Training large models on large datasets takes a long time
  - Would like to use multiple computers to parallelize training
- Different methods for parallelizing across multiple computers
  - **Data**
  - Model
- Different methods for synchronization across multiple computers
  - **Synchronous**
  - Asynchronous



(a) Data Parallelism  
machine1 machine2



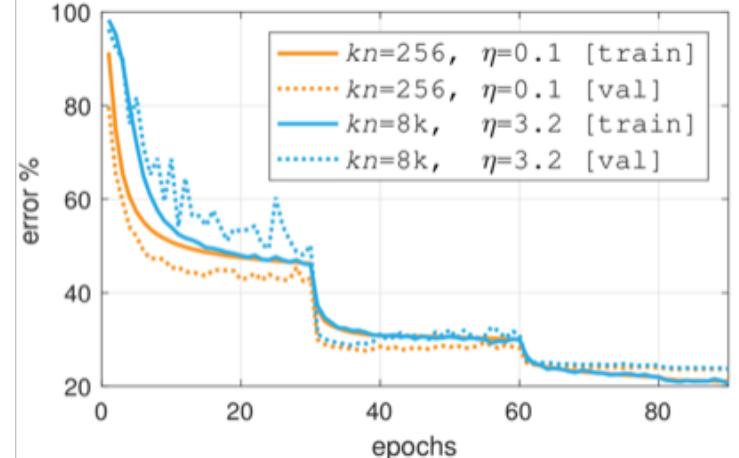
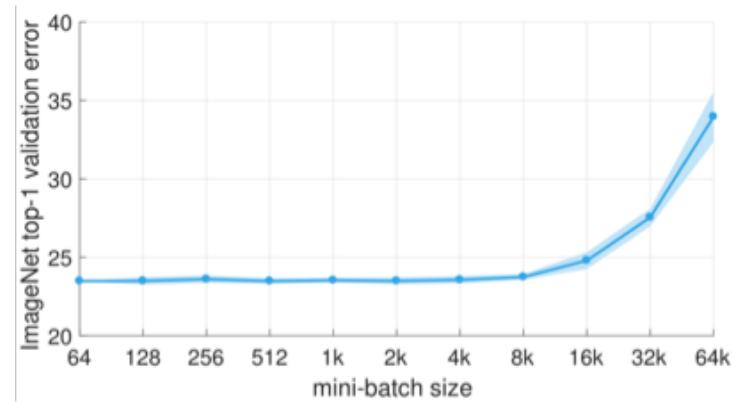
(b) Model Parallelism

# Synchronous Stochastic Gradient Descent

- Synchronous gradient updates
  - Want a large batch size for efficiency
  - Give a part of the larger batch to each worker
  - But a large batch size causes optimization problems
  - Popular benchmark is training ResNet 50 on ImageNet to a specified accuracy
- Accurate, large minibatch SGD: training ImageNet in 1 hour
  - <https://arxiv.org/abs/1706.02677>
- Large batch training of convolutional networks
  - <https://arxiv.org/abs/1708.03888>
- ImageNet training in minutes
  - <https://arxiv.org/abs/1709.05011>
- Extremely large minibatch SGD: training ResNet-50 on ImageNet in 15 minutes
  - <https://arxiv.org/abs/1711.04325>

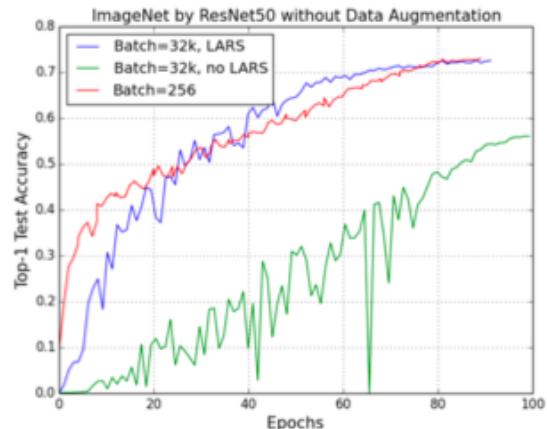
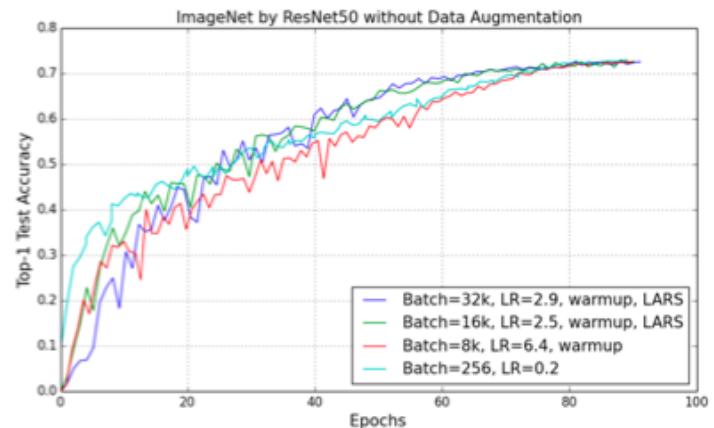
# Batch Size For Parallel

- How to select the batch size for parallel training
  - Comment: ideally want a huge batch size
  - Why? So an arbitrarily large number of workers can all process a serial machine optimal batch size
  - Say serial machine optimal is 32 and the desire is to have 1024 machines in parallel for training, that implies a batch size of 32768
  - Without modification, SGD tends to fail for that case; this observation has motivated a number of SGD modifications
- Accurate, large minibatch SGD: training ImageNet in 1 hour
  - <https://arxiv.org/abs/1706.02677>
  - Used a linear scaling rule to adjust the learning rate (multiply the learning rate by the multiple of the batch size) and used a warm up approach that started the learning rate small in the beginning when the weights were varying the most to allow training with batch sizes up to 8192 image



# Batch Size For Parallel

- Large batch training of convolutional networks
  - <https://arxiv.org/abs/1708.03888>
  - Found that the warm up method didn't work well enough, replaced it with a different learning rate for each layer that allowed training with very large batch sizes
- ImageNet training in minutes
  - <https://arxiv.org/abs/1709.05011>
  - Used the above large batch training algorithm scaled to 1024 nodes and trained ResNet to published accuracy in ~ 15 minutes



# Asynchronous Stochastic Gradient Descent

- Motivation
  - Synchronization of gradient updates introduce a computational bottleneck
  - This can be seen as a feedback system with a tight loop
  - Allow asynchronous updates of the gradients to a common parameter server
  - Challenge is that all gradient updates are based on different models
- Large scale distributed deep networks
  - <https://storage.googleapis.com/pub-tools-public-publication-data/pdf/40565.pdf>
- Asynchronous stochastic gradient descent with delay compensation
  - <https://arxiv.org/abs/1609.08326>

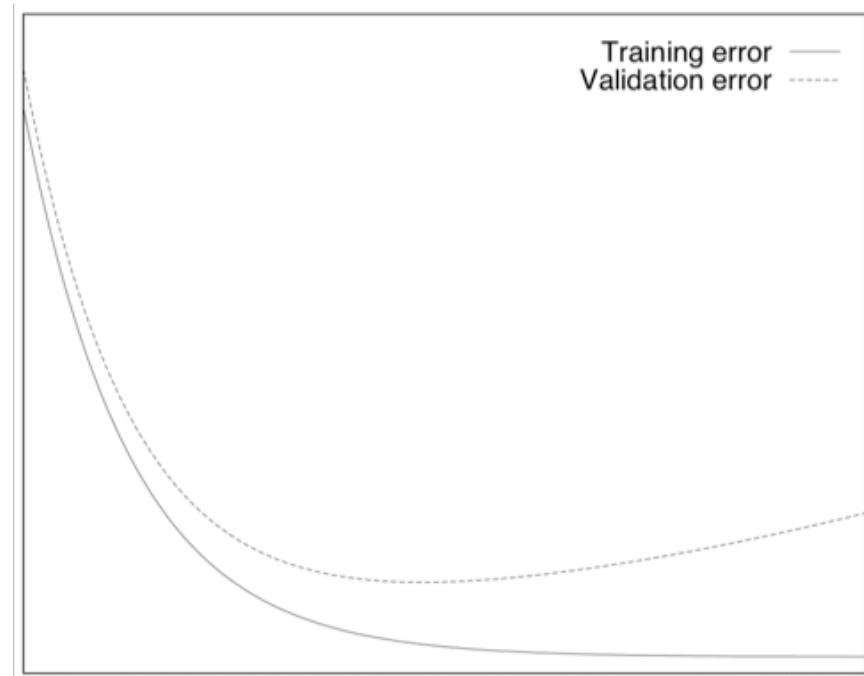
# Evaluation

# Flow

- 2 parts
  - Validation (do this during training)
  - Testing (goal is for this to be good; but can't put it in training loop)

# Validation

- Training length
  - Fixed number of iterations
  - Early stopping criteria based on validation error
- Early stopping - but when?
  - [https://page.mi.fu-berlin.de/prechelt/Biblio/stop\\_tricks1997.pdf](https://page.mi.fu-berlin.de/prechelt/Biblio/stop_tricks1997.pdf)



# Application Specific Evaluation Metrics

- Most evaluation metrics are application specific
  - We'll talk about application specific evaluation metrics in the context of applications
- Speech
  - WER and CER
  - Insertions, deletions, substitutions
  - ...
- Vision
  - Top 1 and top 5 errors for classification
  - ...

# Confusion Matrix

- For 2 classes
  - {True, False} {positive, negative}
  - True and false refer to whether the prediction was correct
  - Positive and negative refer to the predicted value
  - False positive = type 1 error (incorrectly labeled as a member of a class)
  - False negative = type 2 error (incorrectly missed as a member of a class)
- Can generalize to multiple classes
  - Class labels in rows for predicted classes
  - Class labels in cols for actual classes
  - Entries indicate how many in each (predicted, actual) combination
  - Ideally want to see a diagonal matrix

# Precision And Recall

- Precision for a class = number of true positives / (number of true positives + number of false positives)
  - Conceptually
    - Take all the predictions of a particular class
    - The ratio of correct predictions to total predictions is the precision
  - Precision = 1 = every item labeled as belonging to the class actually does belong to the class (but items from the class could have been labeled as belonging to other classes)
- Recall for a class = number of true positives / (number of true positives + number of false negatives)
  - Conceptually
    - Take all the inputs of a particular class
    - The ratio of correct predictions to total inputs is the recall
  - Recall = 1 = every item belonging to the class was labeled as belonging to the class (but items not belonging to the class could also have been labeled as belonging to the class)
  - Also called true positive rate and sensitivity

# Precision And Recall

- Relationship
  - Typically increasing precision decreases recall
  - Typically increasing recall decreases precision
  - As they're linked they're typically reported together
    - Precision at a specific recall (or multiple pairs to form a curve)
      - Upper right is best

# Receiver Operating Characteristic (ROC) Curve

- True positive rate for a class = number of true positives / (number of true positives + number of false negatives)
  - Conceptually
    - Take all the inputs of a particular class
    - The ratio of correct predictions to total inputs is the true positive rate
- False positive rate for a class = number of false positives / (number of false positives + number of true negatives)
  - Conceptually
    - Take all the inputs not of a particular class
    - The ratio of incorrect predictions to total inputs is the false positive rate

# Receiver Operating Characteristic (ROC) Curve

- Relationship
  - Typically increasing the true positive rate also increases the false positive rate
  - Typically decreasing the false positive rate also decreases the true positive rate
  - As they're linked they're typically reported together
    - True positive rate at a specified false positive rate
    - Upper left is best

# Testing

- Remember: danger of putting final testing in the same loop (frequently implicitly)

# Hyper Parameter Selection

# How You Configure Training

- This effectively how you configure the training
  - But it's listed here at the end of the training presentation to allow the previous sections to introduce all the different parameters first
- How do you choose values?
  - Start from good settings that someone else found for a similar problem
  - Maybe modify them a little
  - Do some sort of search (grid, random, ...) with a bunch of test trainings
  - Max out some of the parameters until you hit divergence, then back off a bit
  - ...

# Examples

- Data
  - Batch size and selection
  - Pre processing
- Initialization
  - Distribution
- Forward pass

# Examples Continued

- Error calculation
  - Loss function
- Weight update method and schedule
  - Stochastic gradient descent variant
  - Learning rate
  - Weight decay
- Evaluation
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# Evaluation

# Hyper Parameter Selection