Lecture 11:
Training Neural Networks
(Part 2)

Reminder: A3

Due this Friday 10/9 at 11:59pm EST

Reminder: 100% on autograder does not mean 100% score! Some components of each assignment will be hand-graded.

Midterm

- Monday, October 19
- Will be online via https://crabster.org/
- Exam is 90 minutes
- You can take it any time in a 24-hour window
- We will have 3-4 "on-call" periods during the 24-hour window where GSIs will answer questions within ~15 minutes
- Open note
- True / False, multiple choice, short answer
- For short answer questions requiring math, either write LaTeX or upload an image with handwritten math

Overview

1. **One time setup**
   Activation functions, data preprocessing, weight initialization, regularization

Last Time

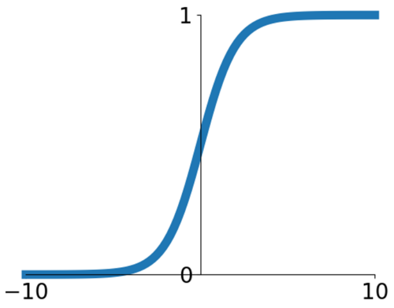
2. **Training dynamics**
   Learning rate schedules; hyperparameter optimization
3. **After training**
   Model ensembles, transfer learning, large-batch training

Today

Last Time: Activation Functions

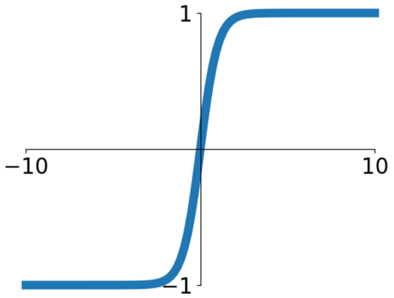
Sigmoid

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



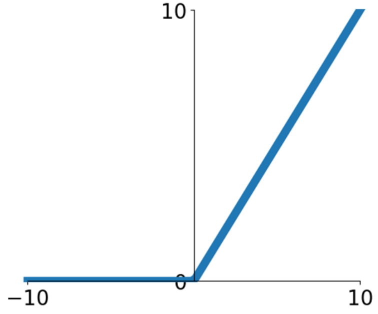
tanh

$$\tanh(x)$$



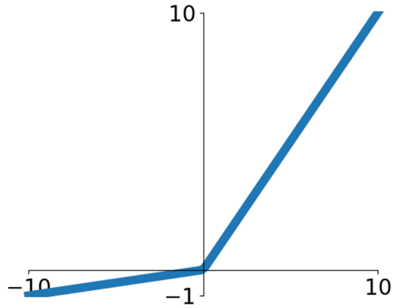
ReLU

$$\max(0, x)$$



Leaky ReLU

$$\max(0.1x, x)$$

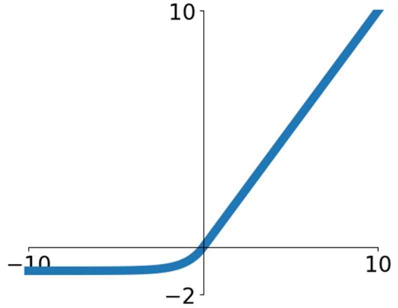


Maxout

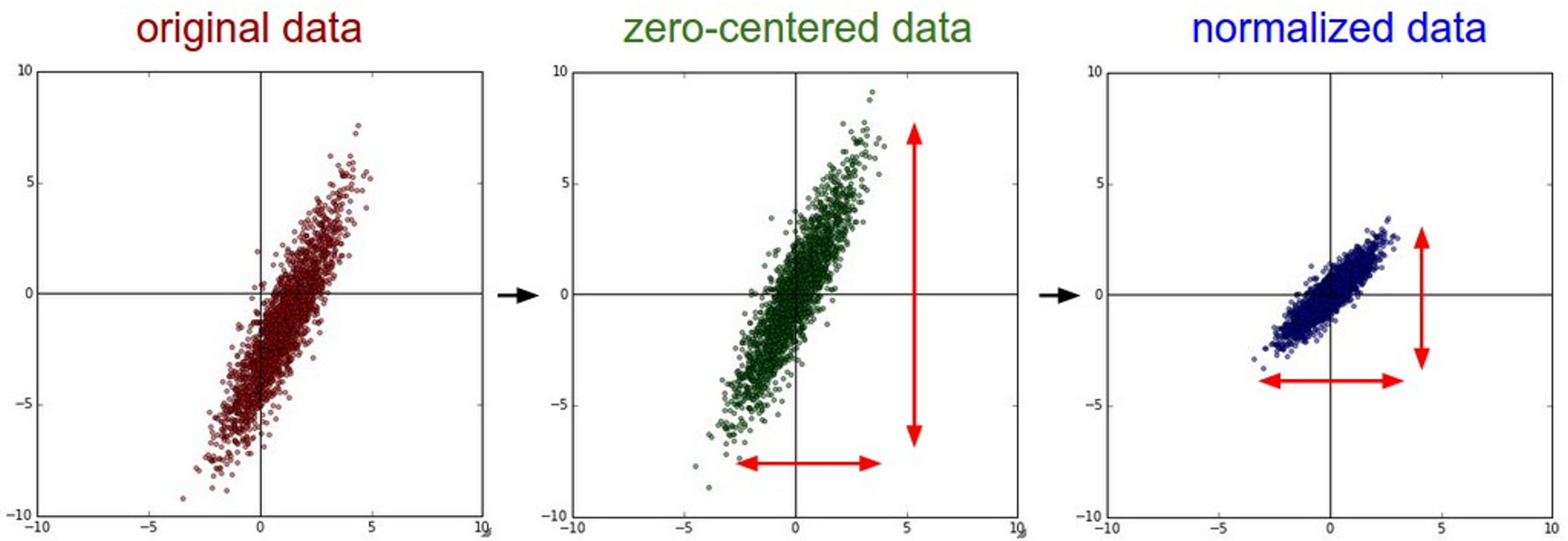
$$\max(w_1^T x + b_1, w_2^T x + b_2)$$

ELU

$$\begin{cases} x & x \geq 0 \\ \alpha(e^x - 1) & x < 0 \end{cases}$$



Last Time: Data Preprocessing

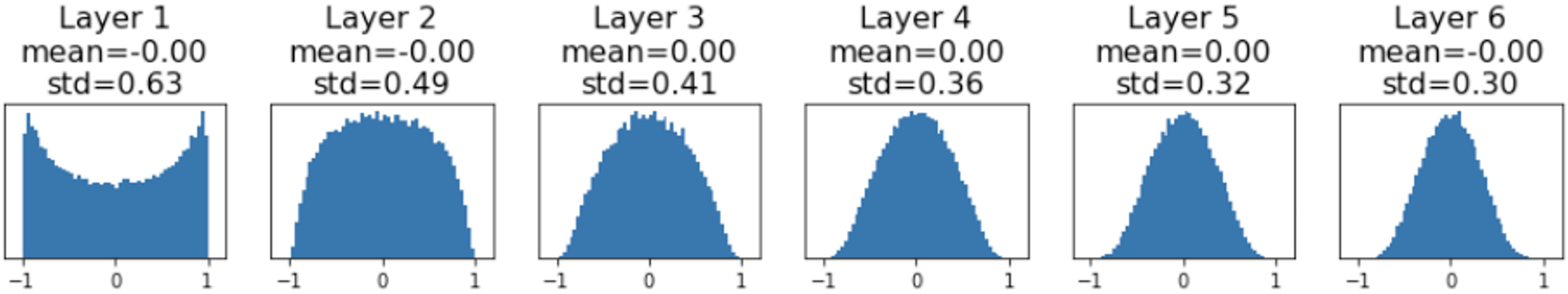


Last Time: Weight Initialization

```python
dims = [4096] * 7
hs = []
x = np.random.randn(16, dims[0])
for Din, Dout in zip(dims[:-1], dims[1:]):
    W = np.random.randn(Din, Dout) / np.sqrt(Din)
    x = np.tanh(x.dot(W))
    hs.append(x)
```

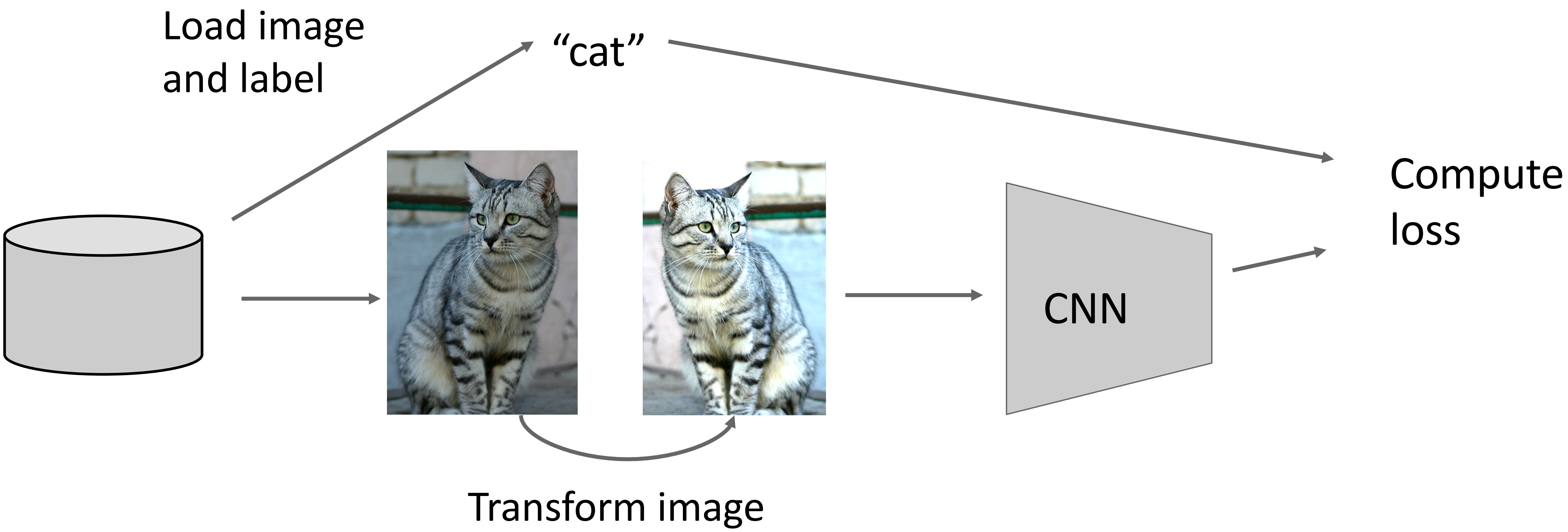
"Xavier" initialization:
std = 1/sqrt(Din)

"Just right": Activations are nicely scaled for all layers!



Glorot and Bengio, "Understanding the difficulty of training deep feedforward neural networks", AISTAT 2010

Last Time: Data Augmentation

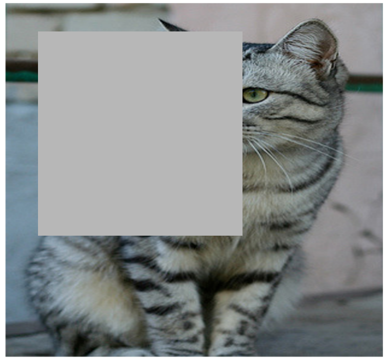


Last Time: Regularization

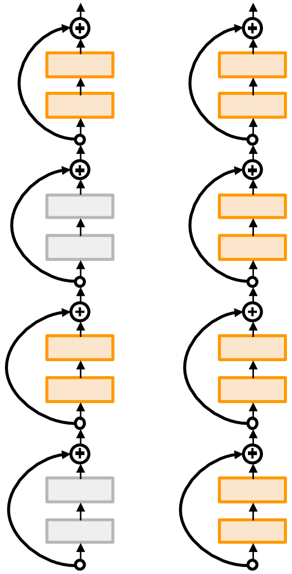
Training: Add randomness
Testing: Marginalize out randomness

Examples:
Batch Normalization
Data Augmentation

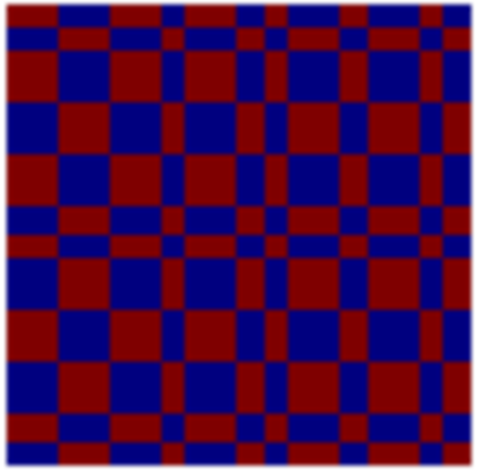
Cutout



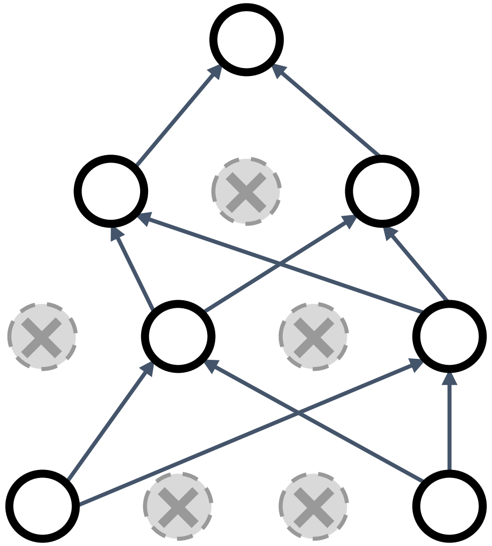
Stochastic Depth



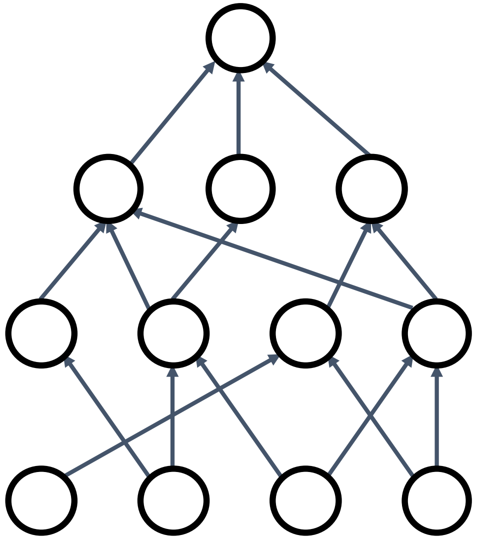
Fractional pooling



Dropout



DropConnect



Mixup

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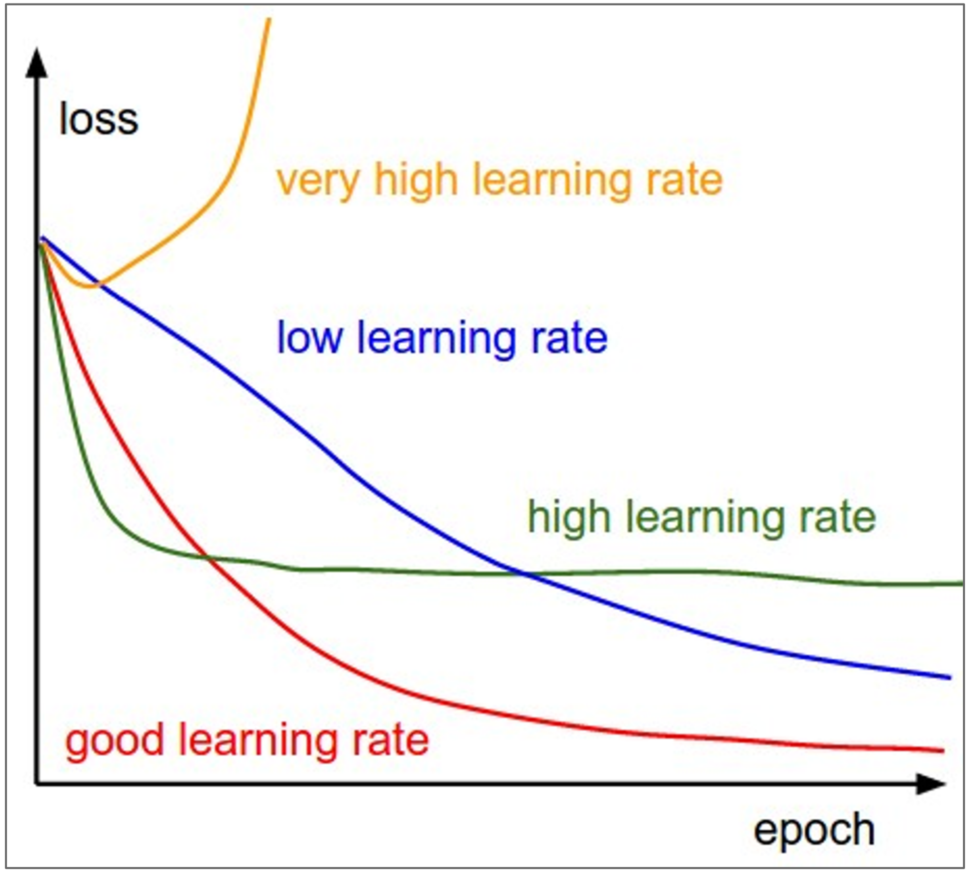
Today

Learning Rate Schedules

SGD, SGD+Momentum, Adagrad, RMSProp, Adam all have **learning rate** as a hyperparameter.



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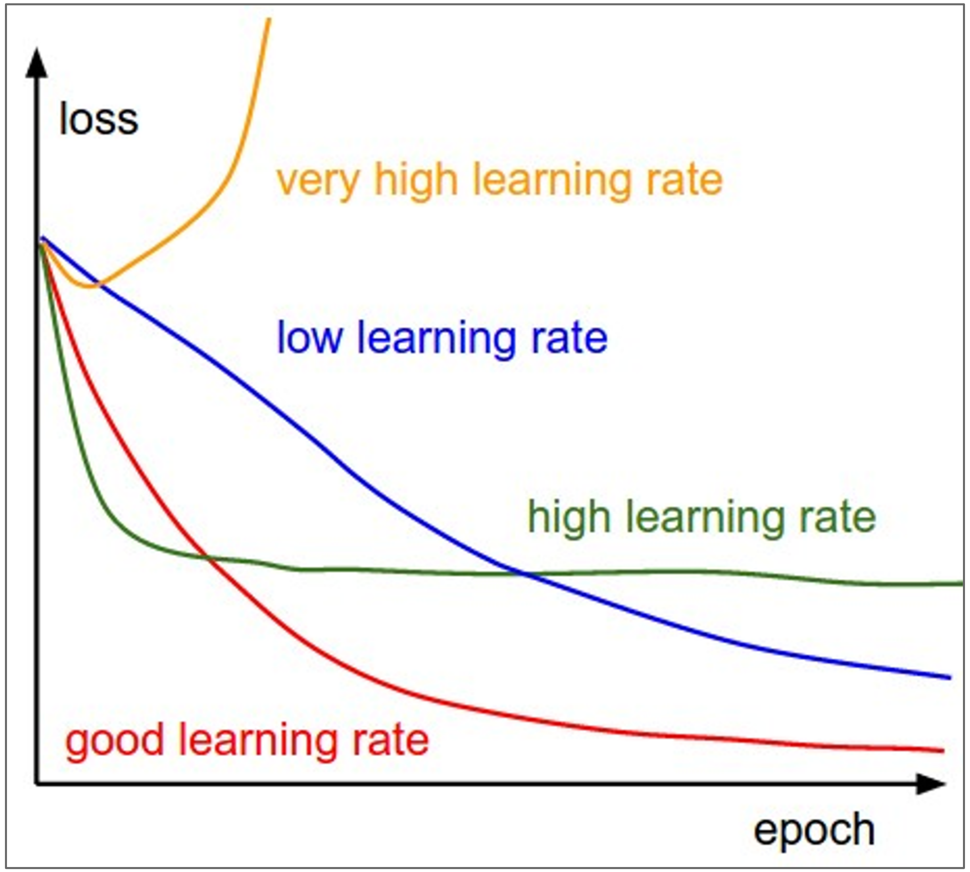
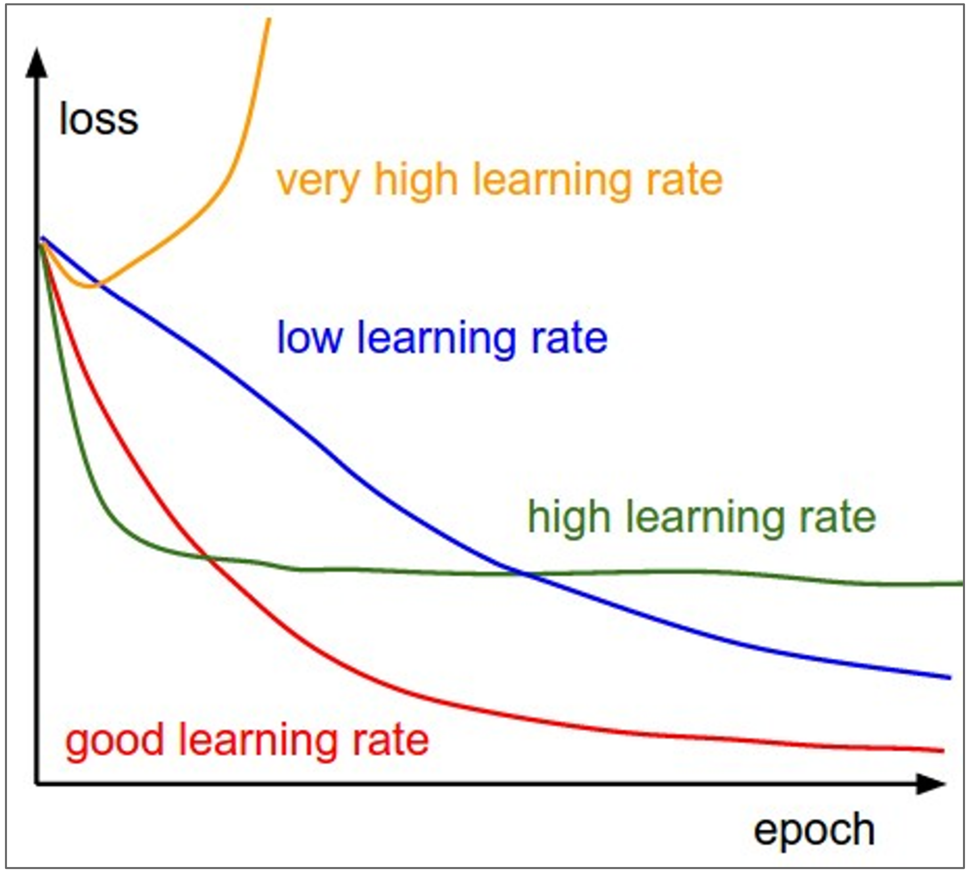


Q: Which one of these learning rates is best to use?

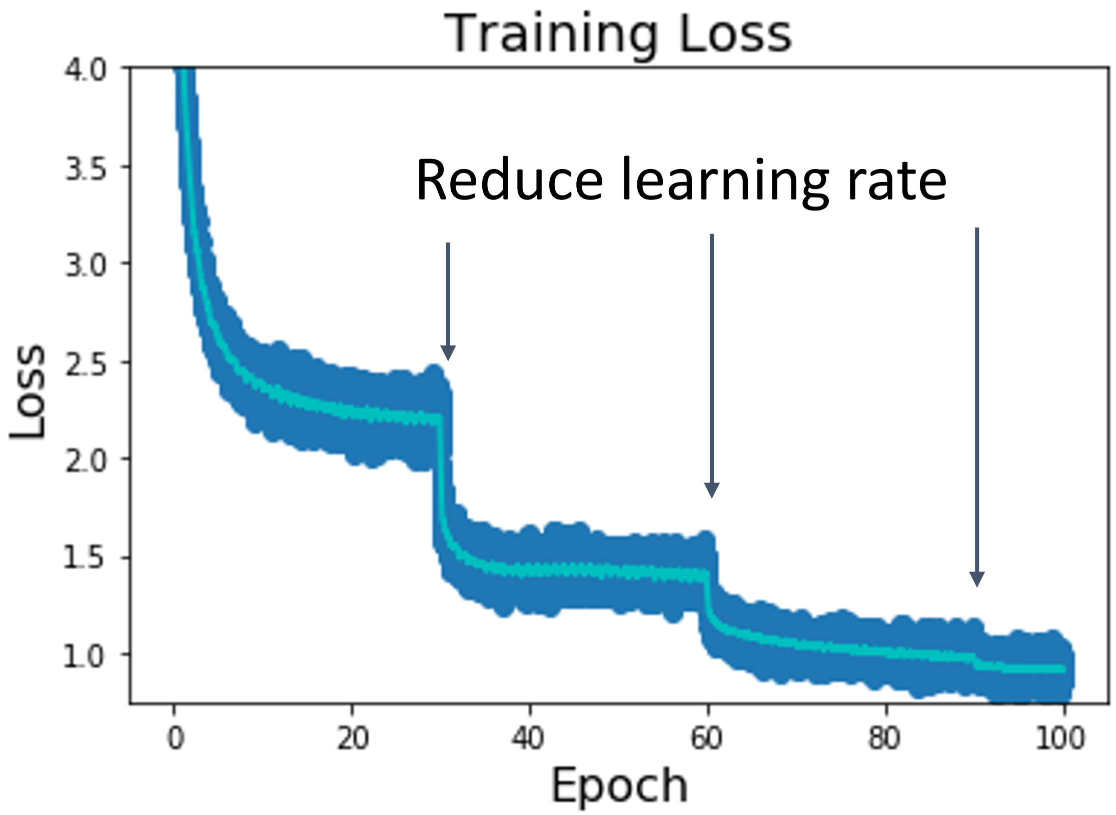
SGD, SGD+Momentum, Adagrad, RMSProp, Adam
all have **learning rate** as a hyperparameter.



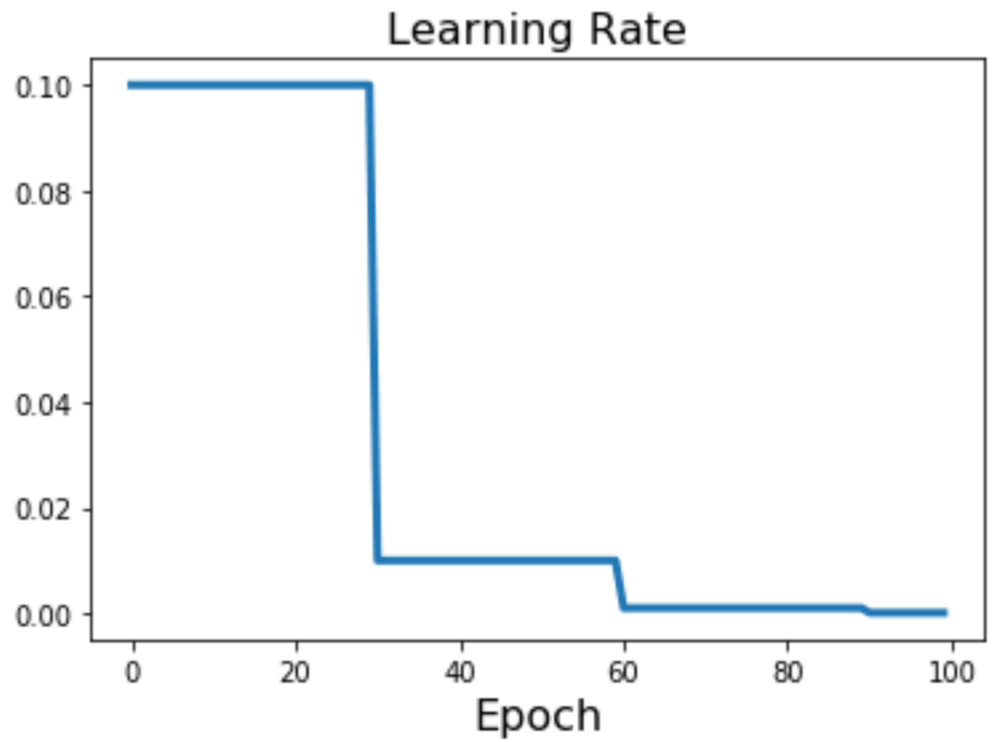
Q: Which one of these learning rates is best to use?

A: All of them! Start with large learning rate and decay over time

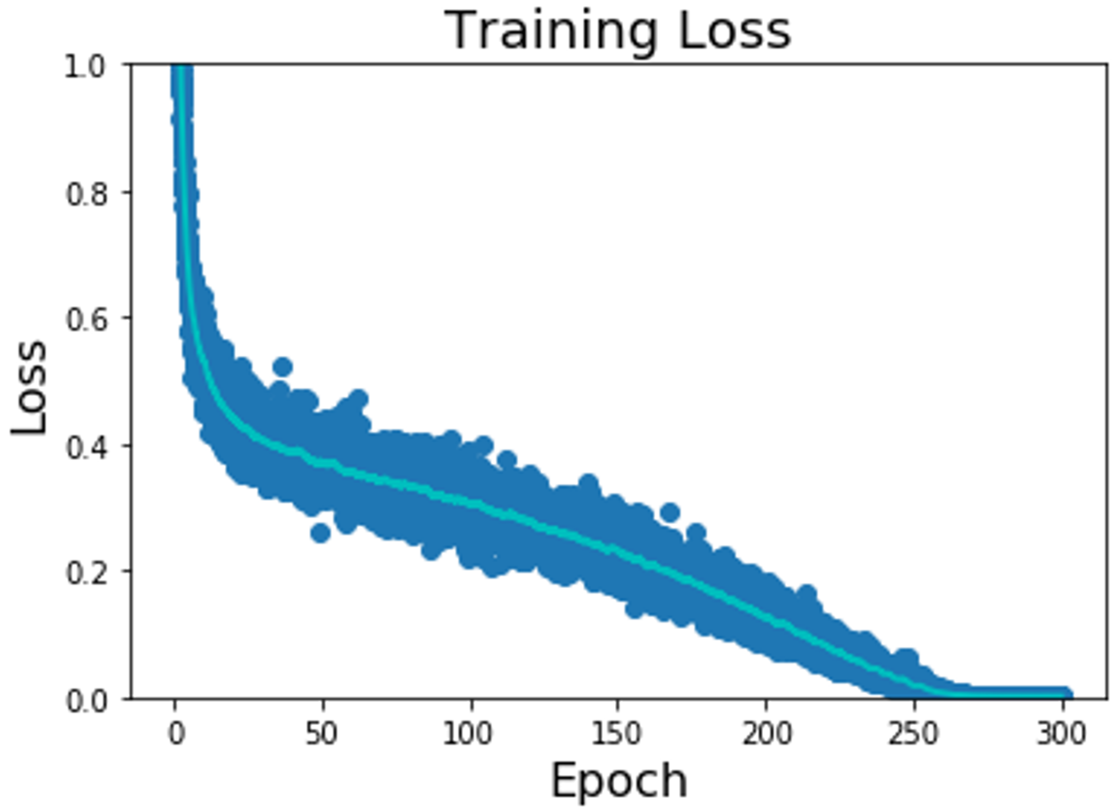
Learning Rate Decay: Step



Step: Reduce learning rate at a few fixed points. E.g. for ResNets, multiply LR by 0.1 after epochs 30, 60, and 90.

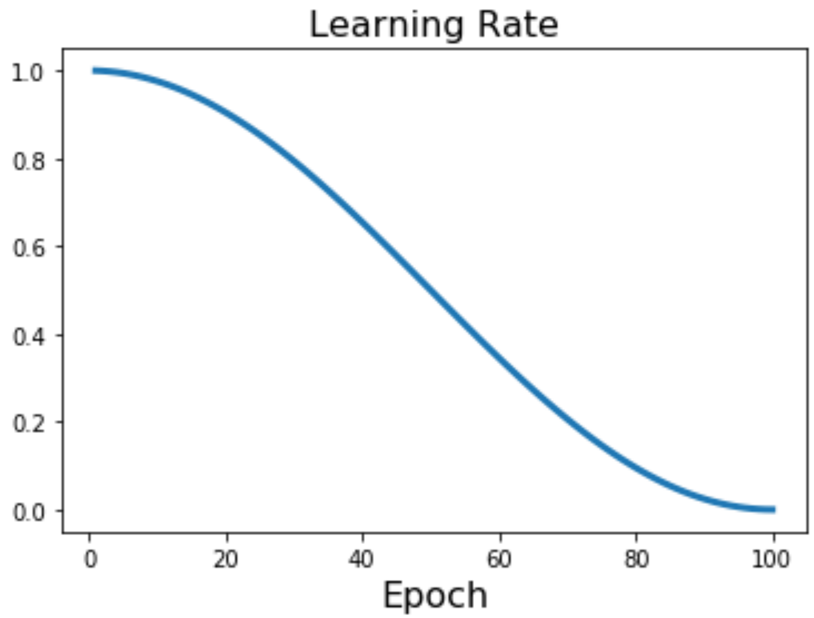


Learning Rate Decay: Cosine



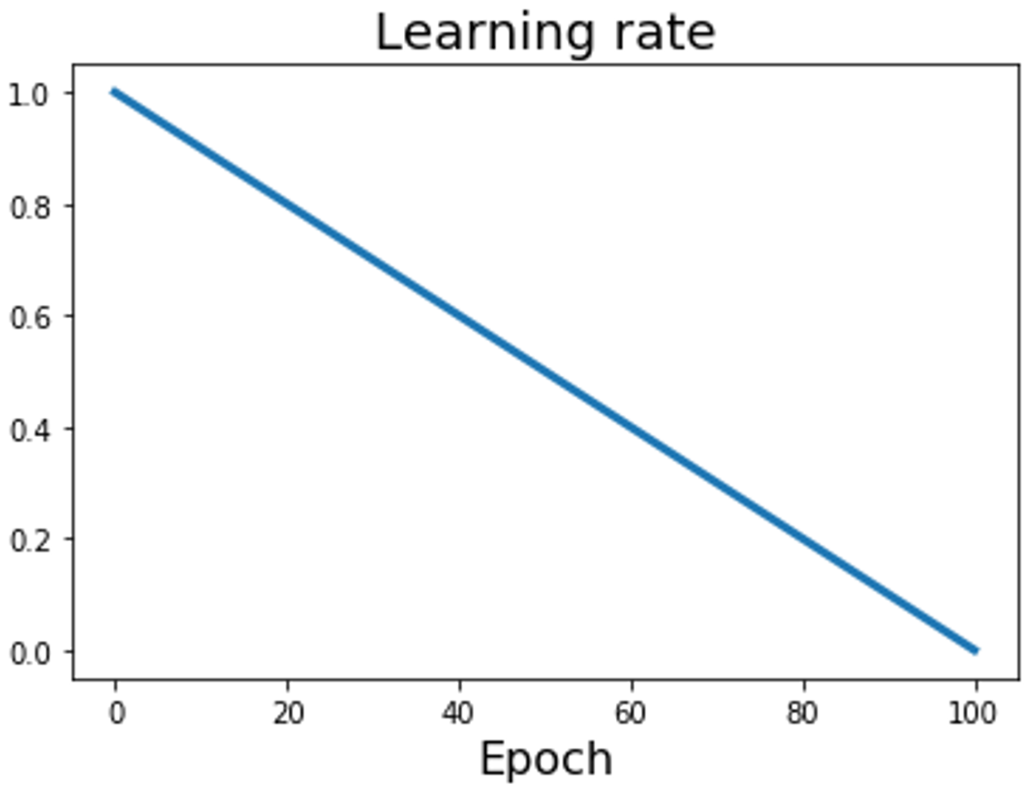
Step: Reduce learning rate at a few fixed points. E.g. for ResNets, multiply LR by 0.1 after epochs 30, 60, and 90.

Cosine: $$\alpha_t = \frac{1}{2}\alpha_0\left(1+\cos\left(\frac{t\pi}{T}\right)\right)$$



Loshchilov and Hutter, "SGDR: Stochastic Gradient Descent with Warm Restarts", ICLR 2017
Radford et al, "Improving Language Understanding by Generative Pre-Training", 2018
Feichtenhofer et al, "SlowFast Networks for Video Recognition", ICCV 2019
Radosavovic et al, "On Network Design Spaces for Visual Recognition", ICCV 2019
Child at al, "Generating Long Sequences with Sparse Transformers", arXiv 2019

Learning Rate Decay: Linear



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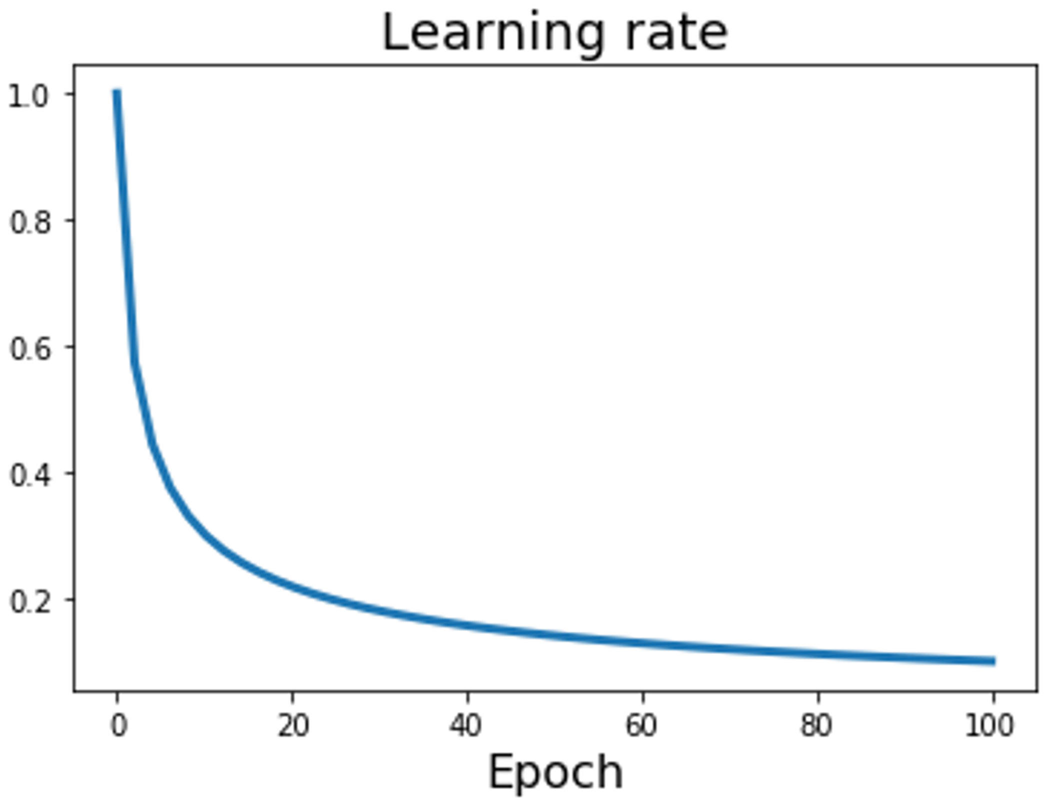
Cosine: $$\alpha_t = \frac{1}{2}\alpha_0\left(1 + \cos\left(\frac{t\pi}{T}\right)\right)$$

Linear: $$\alpha_t = \alpha_0\left(1 - \frac{t}{T}\right)$$

Devlin et al, "BERT: Pre-training of Deep Bidirectional Transformers for Language Understanding", NAACL 2018
Liu et al, "RoBERTa: A Robustly Optimized BERT Pretraining Approach", 2019
Yang et al, "XLNet: Generalized Autoregressive Pretraining for Language Understanding", NeurIPS 2019

Learning Rate Decay: Inverse Sqrt



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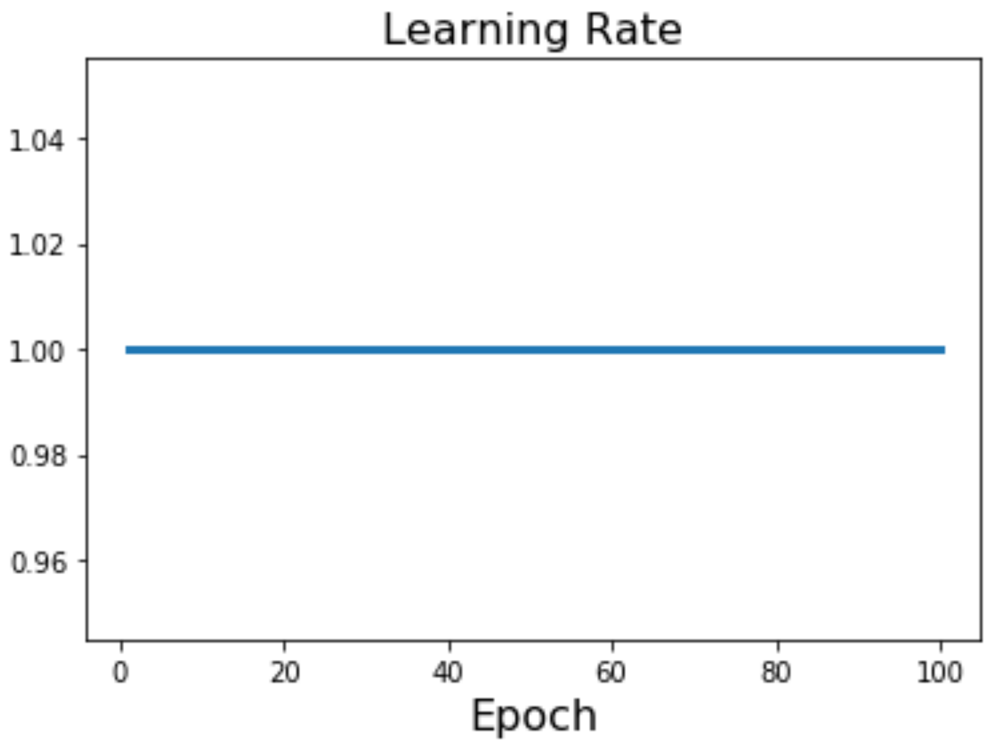
Linear: $$\alpha_t = \alpha_0\left(1 - \frac{t}{T}\right)$$

Inverse sqrt: $$\alpha_t = \alpha_0/\sqrt{t}$$

Vaswani et al, "Attention is all you need", NIPS 2017

Learning Rate Decay: Constant!



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Cosine: $\alpha_t = \frac{1}{2}\alpha_0\left(1 + \cos\left(\frac{t\pi}{T}\right)\right)$

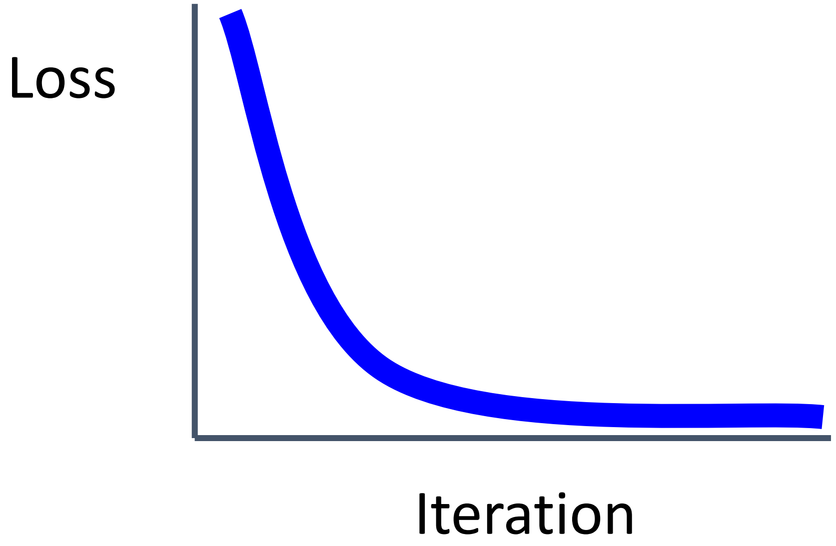
Linear: $\alpha_t = \alpha_0\left(1 - \frac{t}{T}\right)$

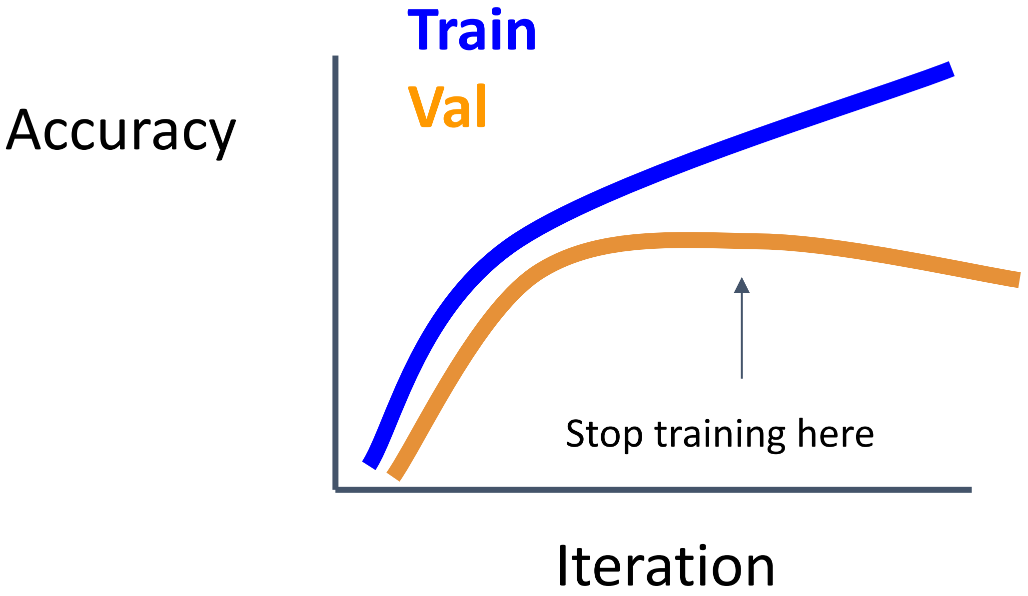
Inverse sqrt: $\alpha_t = \alpha_0/\sqrt{t}$

Constant: $\alpha_t = \alpha_0$

Brock et al, "Large Scale GAN Training for High Fidelity Natural Image Synthesis", ICLR 2019
Donahue and Simonyan, "Large Scale Adversarial Representation Learning", NeurIPS 2019

How long to train? **Early Stopping**





Stop training the model when accuracy on the validation set decreases
Or train for a long time, but always keep track of the model snapshot that worked best on val. **Always a good idea to do this!**

Choosing Hyperparameters

Choosing Hyperparameters: Grid Search

Choose several values for each hyperparameter
(Often space choices log-linearly)

Example:
Weight decay: [$1\text{x}10^{-4}$, $1\text{x}10^{-3}$, $1\text{x}10^{-2}$, $1\text{x}10^{-1}$]
Learning rate: [$1\text{x}10^{-4}$, $1\text{x}10^{-3}$, $1\text{x}10^{-2}$, $1\text{x}10^{-1}$]

Evaluate all possible choices on this
hyperparameter grid

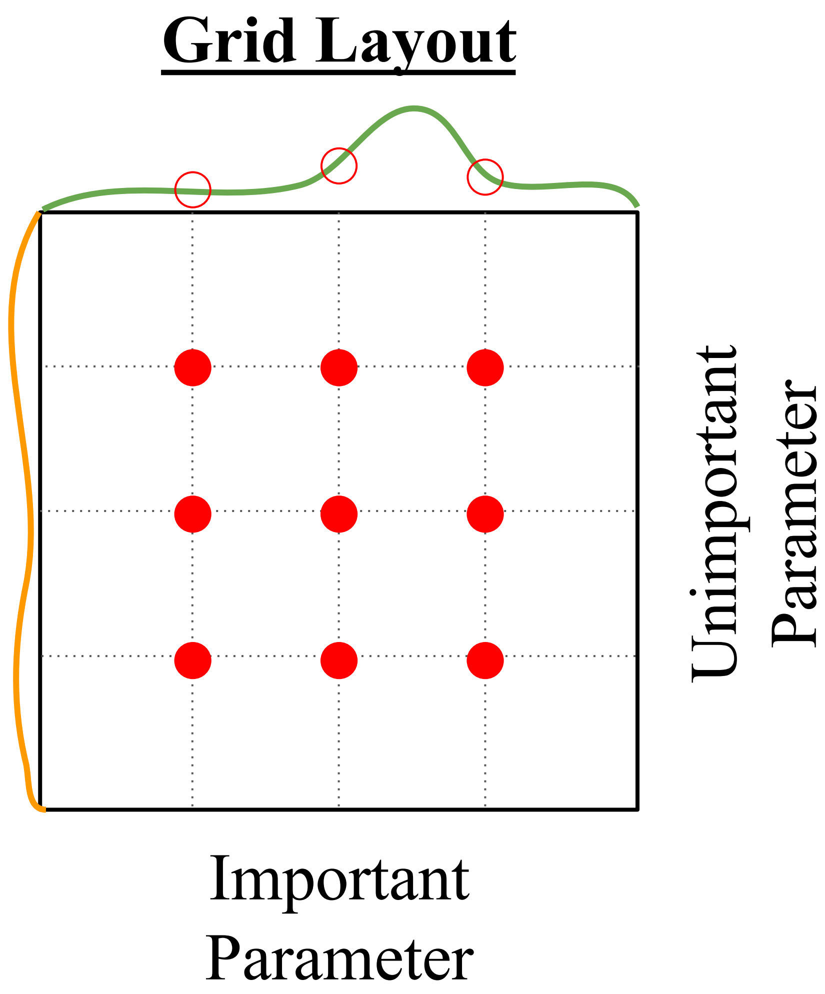
Choosing Hyperparameters: Random Search

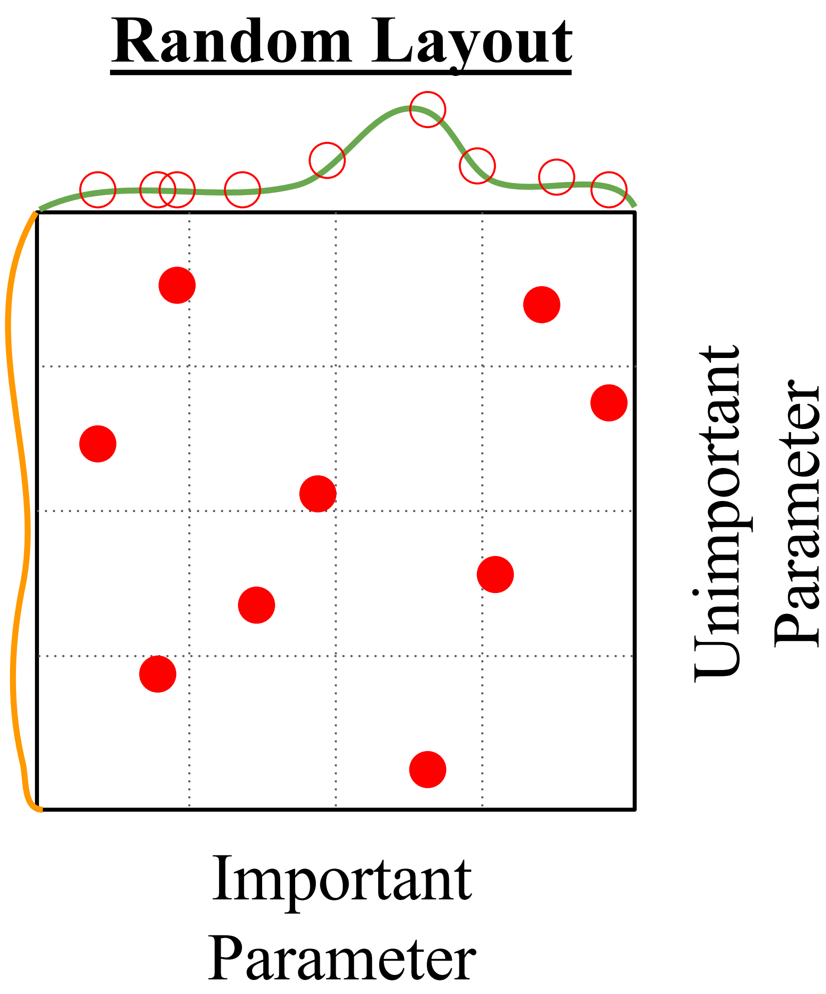
Choose several values for each hyperparameter
(Often space choices log-linearly)

Example:
Weight decay: log-uniform on $[1 \times 10^{-4}, 1 \times 10^{-1}]$
Learning rate: log-uniform on $[1 \times 10^{-4}, 1 \times 10^{-1}]$

Run many different trials

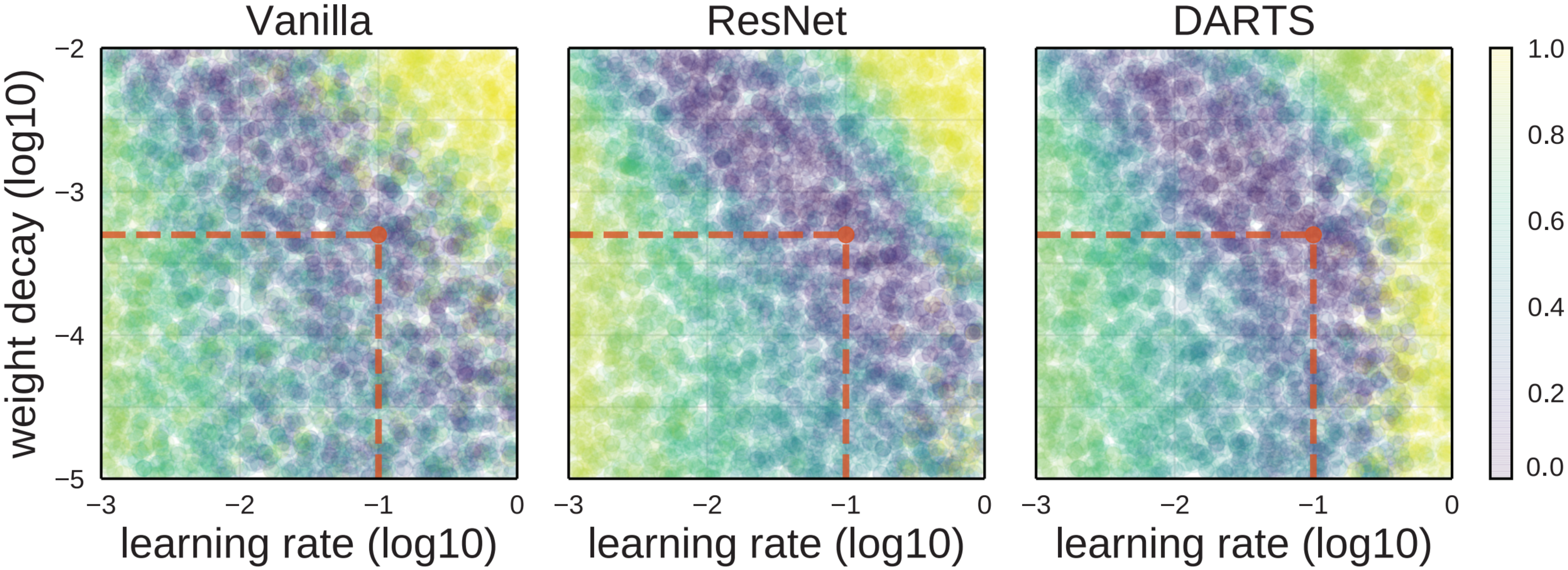
Hyperparameters: Random vs Grid Search





Bergstra and Bengio, “Random Search for Hyper-Parameter Optimization”, JMLR 2012

Choosing Hyperparameters: Random Search



Radosavovic et al, "On Network Design Spaces for Visual Recognition", ICCV 2019

Choosing Hyperparameters

(without tons of GPUs)

Choosing Hyperparameters

Step 1: Check initial loss

Turn off weight decay, sanity check loss at initialization
e.g. log(C) for softmax with C classes

Choosing Hyperparameters

Step 1: Check initial loss
Step 2: Overfit a small sample

Try to train to 100% training accuracy on a small sample of training data (~5-10 minibatches); fiddle with architecture, learning rate, weight initialization. Turn off regularization.

Loss not going down? LR too low, bad initialization
Loss explodes to Inf or NaN? LR too high, bad initialization

Choosing Hyperparameters

Step 1: Check initial loss
Step 2: Overfit a small sample
Step 3: Find LR that makes loss go down

Use the architecture from the previous step, use all training data, turn on small weight decay, find a learning rate that makes the loss drop significantly within ~100 iterations

Good learning rates to try: 1e-1, 1e-2, 1e-3, 1e-4

Choosing Hyperparameters

Step 1: Check initial loss
Step 2: Overfit a small sample
Step 3: Find LR that makes loss go down
Step 4: Coarse grid, train for ~1-5 epochs

Choose a few values of learning rate and weight decay around what worked from Step 3, train a few models for ~1-5 epochs.

Good weight decay to try: 1e-4, 1e-5, 0

Choosing Hyperparameters

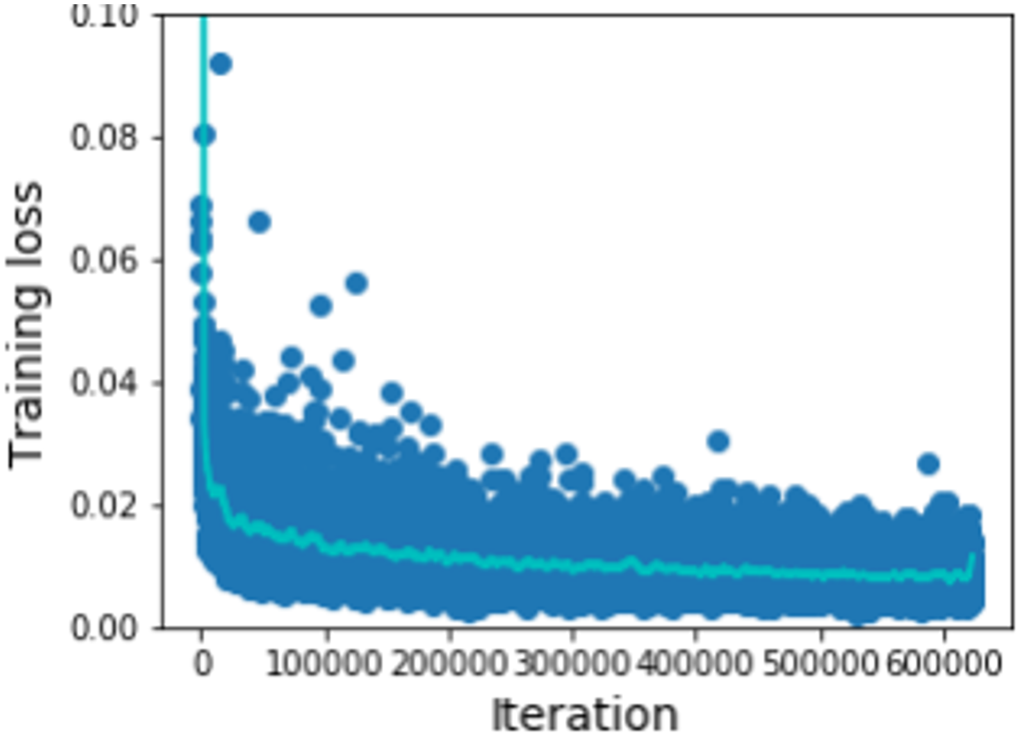
Step 1: Check initial loss
Step 2: Overfit a small sample
Step 3: Find LR that makes loss go down
Step 4: Coarse grid, train for ~1-5 epochs
Step 5: Refine grid, train longer

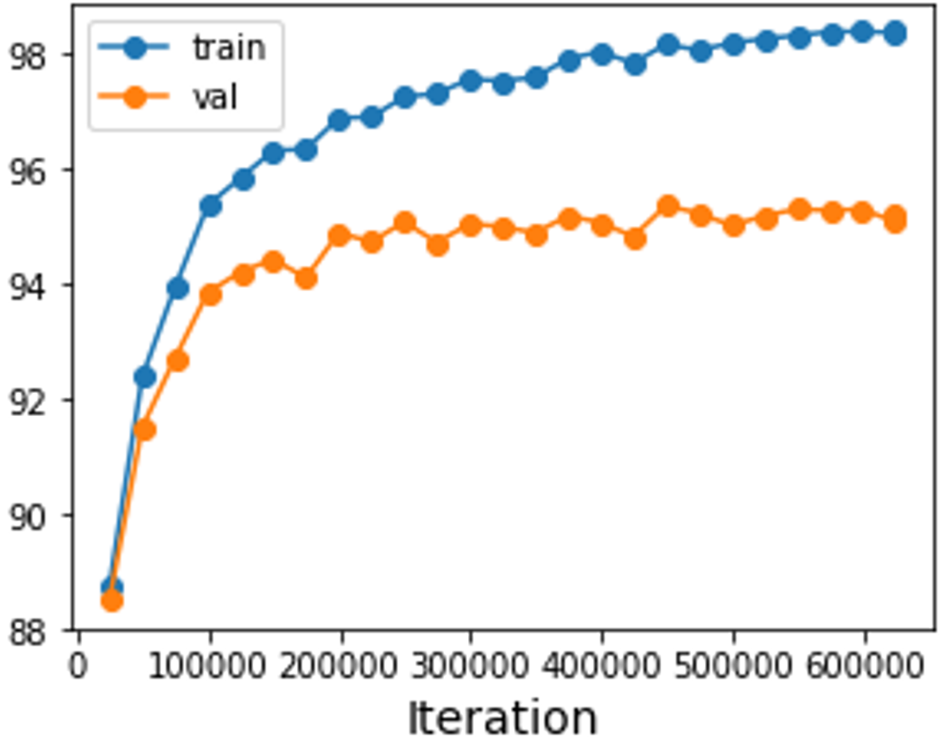
Pick best models from Step 4, train them for longer (~10-20 epochs) without learning rate decay

Choosing Hyperparameters

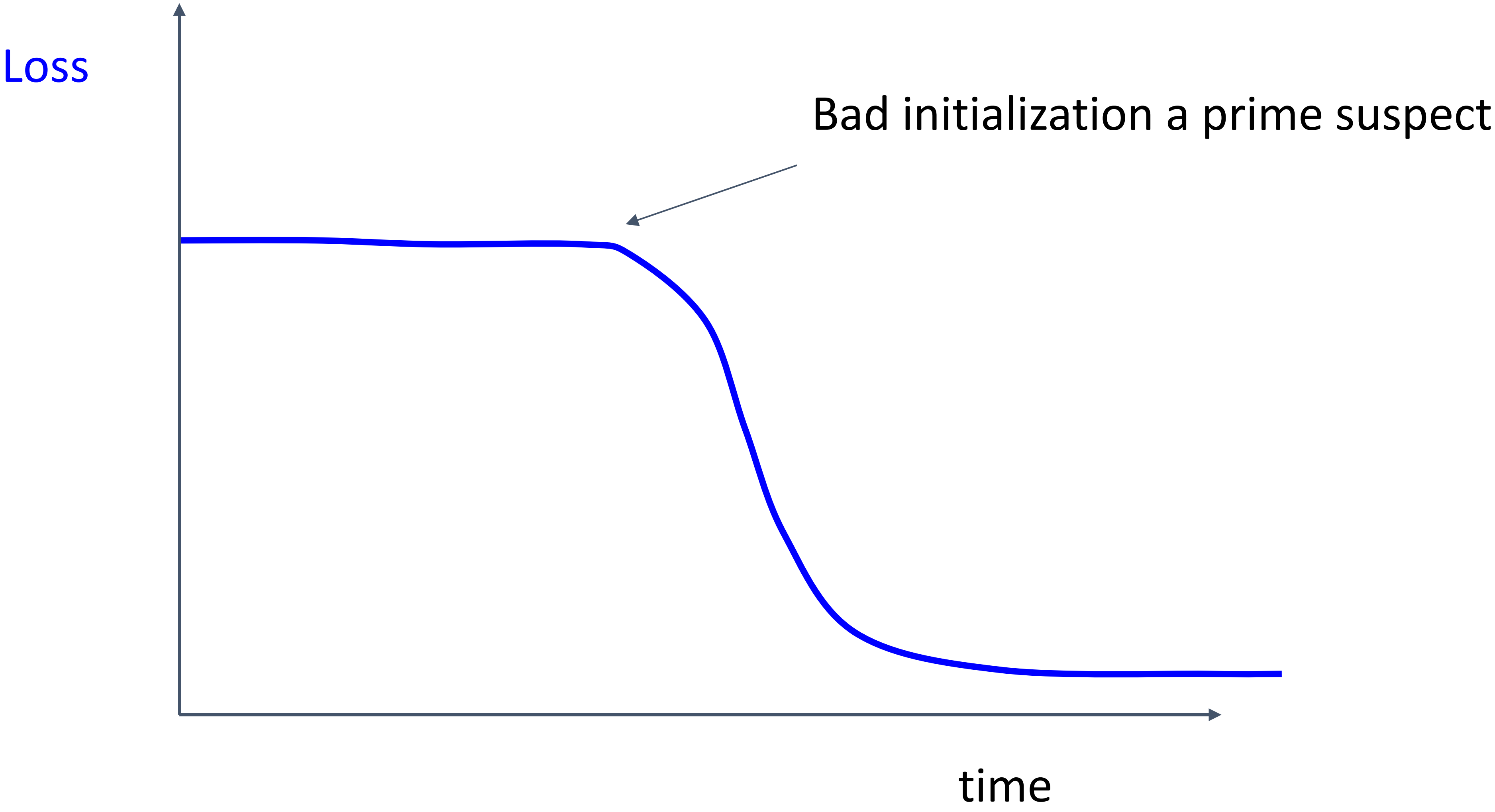
Step 1: Check initial loss
Step 2: Overfit a small sample
Step 3: Find LR that makes loss go down
Step 4: Coarse grid, train for ~1-5 epochs
Step 5: Refine grid, train longer
Step 6: Look at learning curves

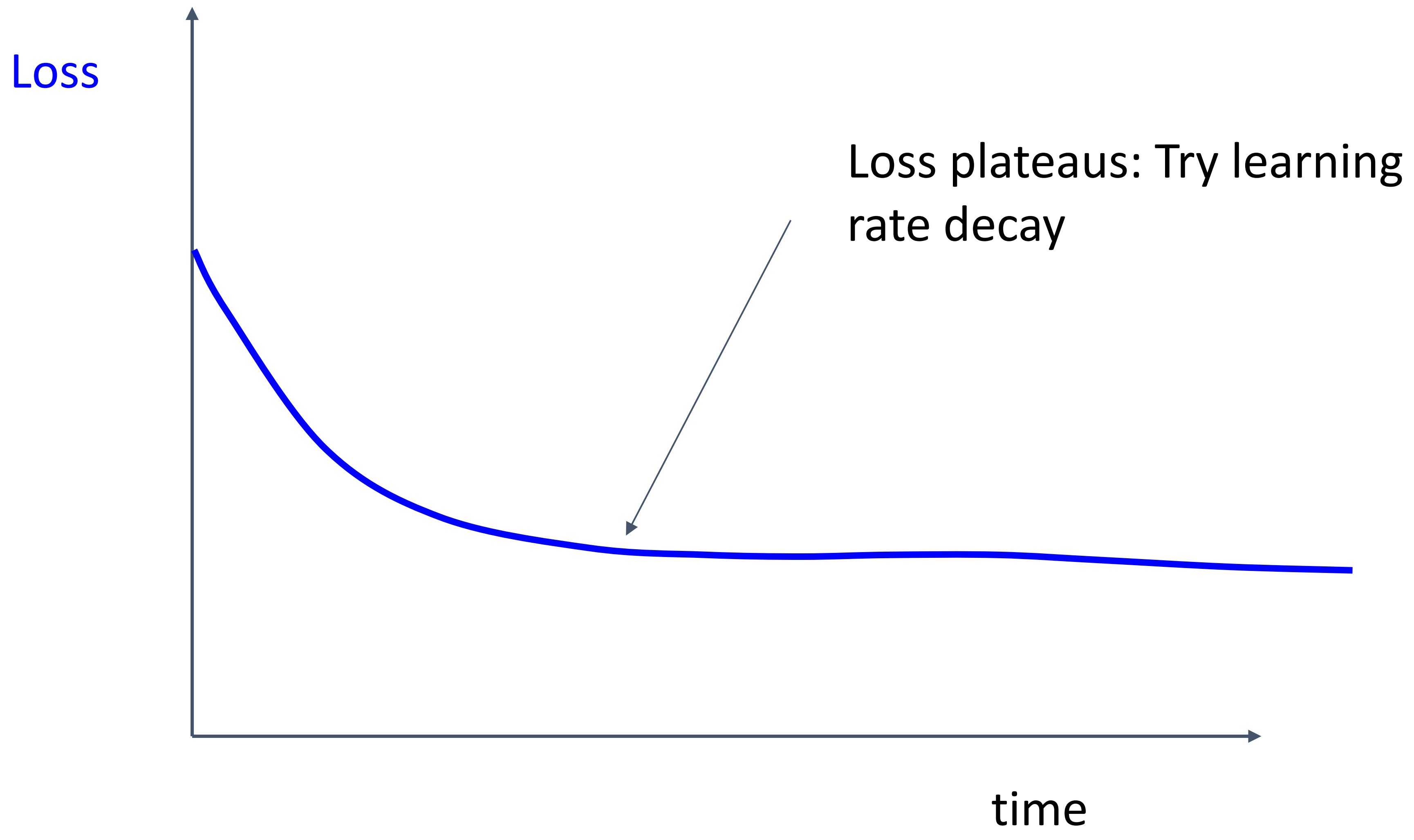
Look at Learning Curves!

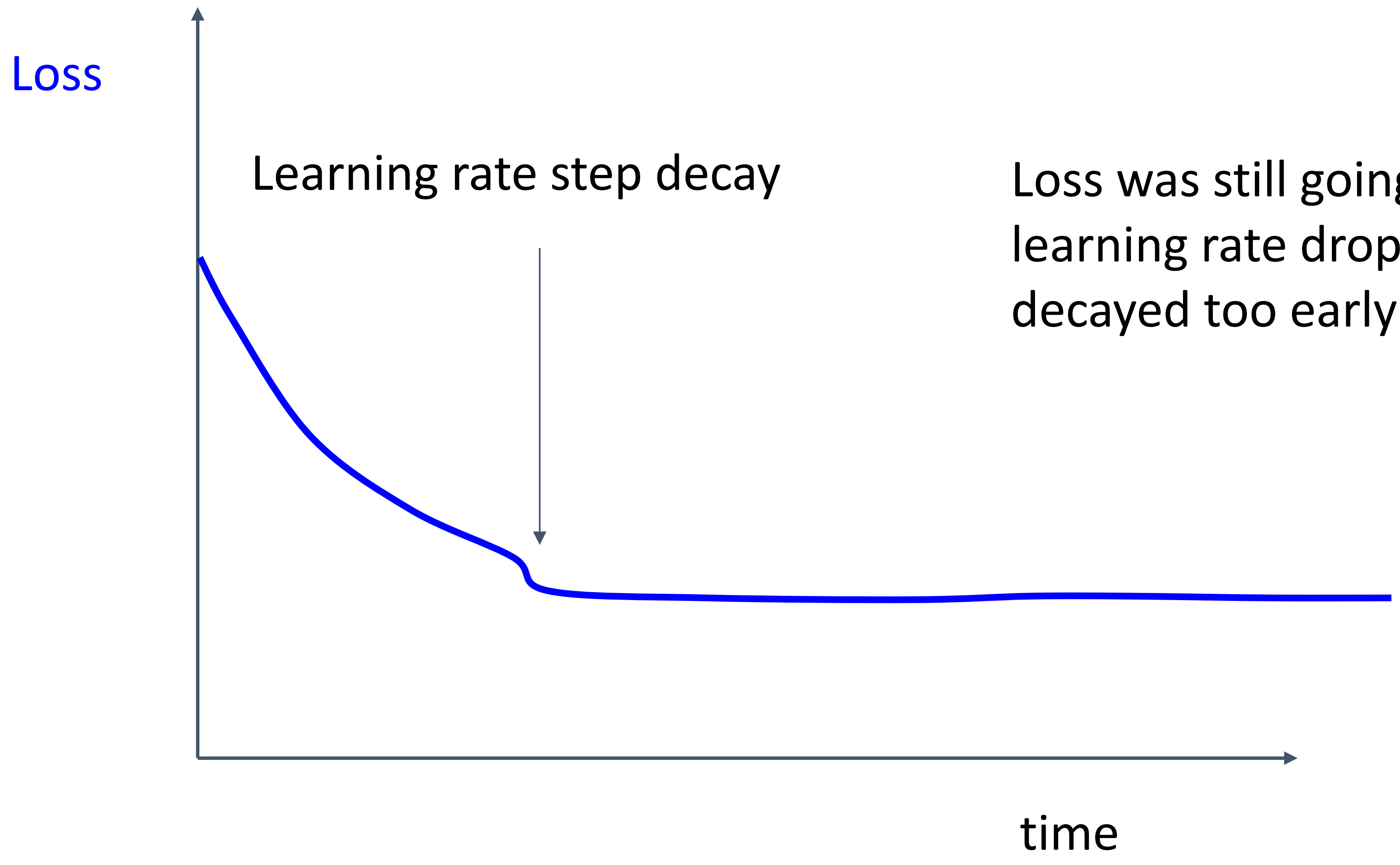




Losses may be noisy, use a scatter plot and also plot moving average to see trends better

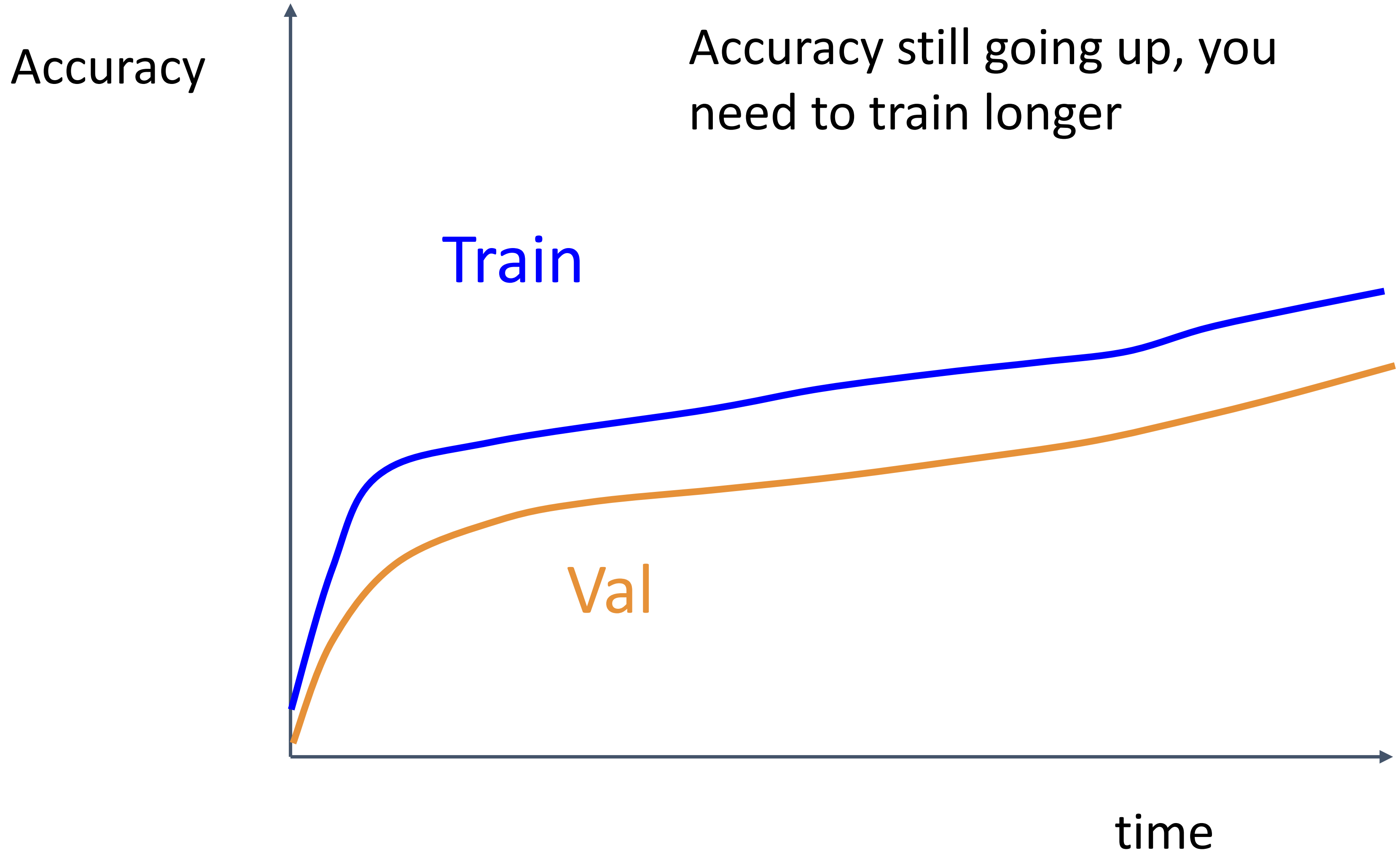

Loss
Bad initialization a prime suspect
time


Loss
Loss plateaus: Try learning rate decay
time

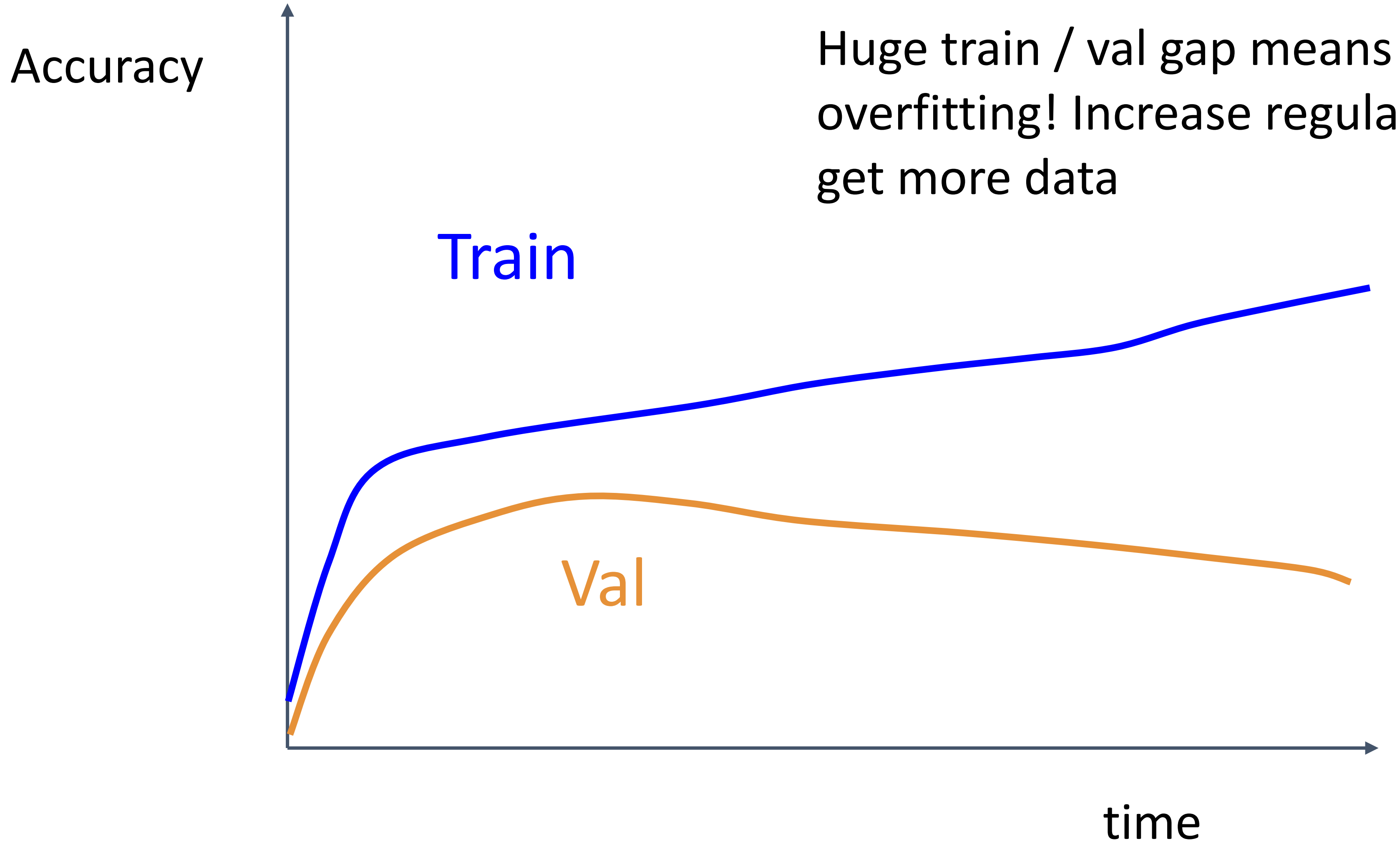


Loss was still going down when learning rate dropped, you decayed too early!

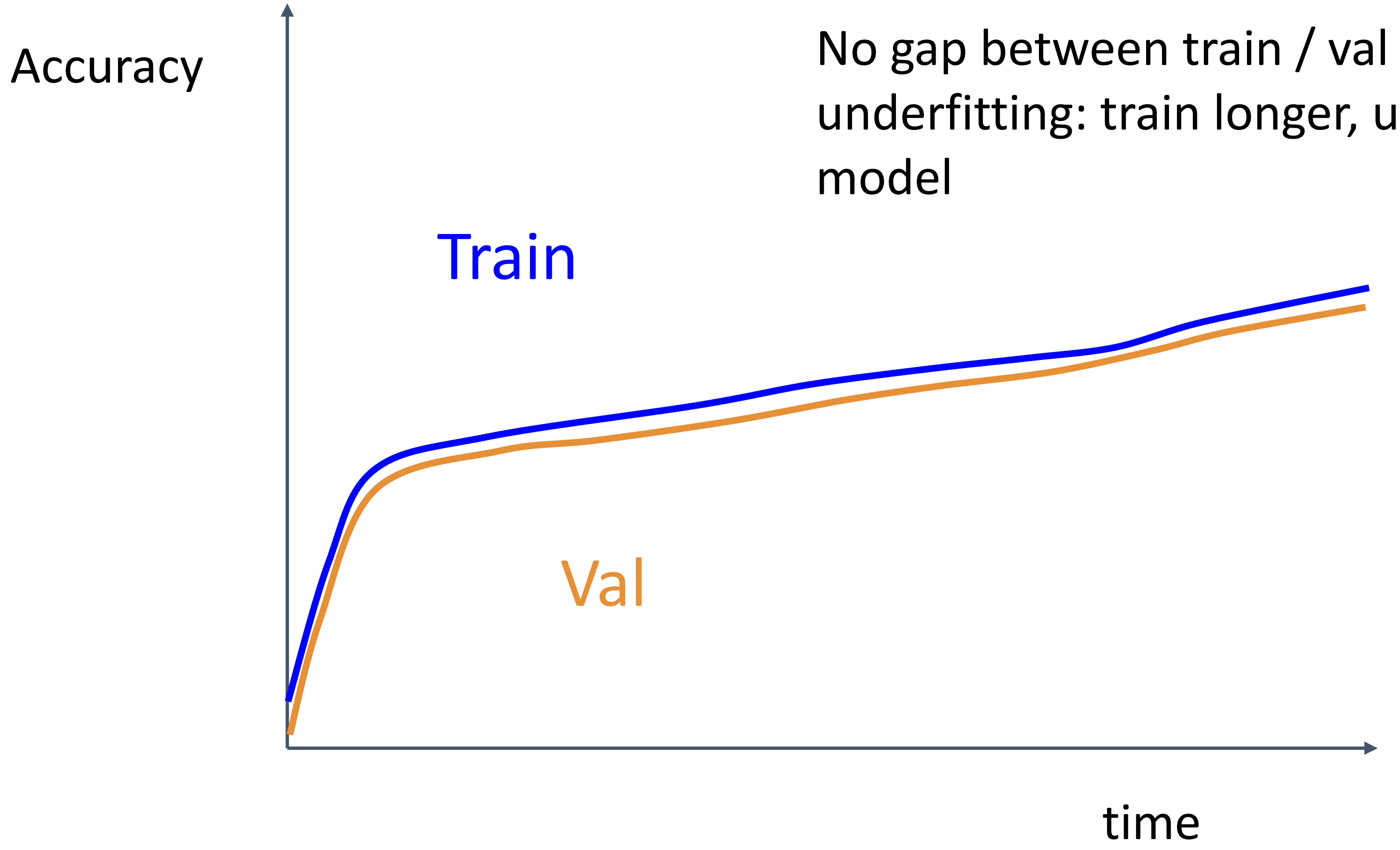
Accuracy still going up, you need to train longer



Huge train / val gap means overfitting! Increase regularization, get more data



No gap between train / val means underfitting: train longer, use a bigger model



Choosing Hyperparameters

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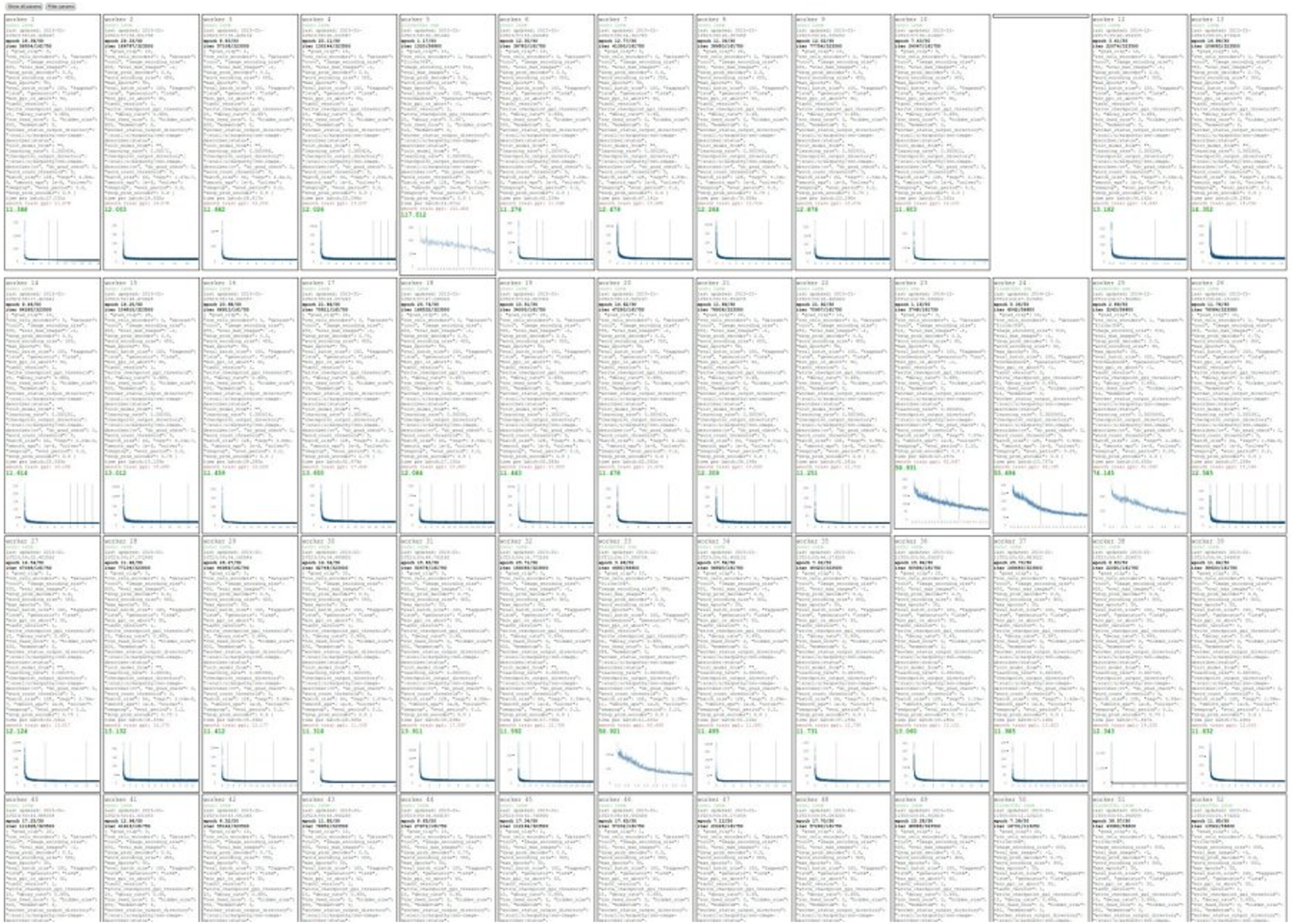
Step 5: Refine grid, train longer
Step 6: Look at loss curves
Step 7: GOTO step 5

Hyperparameters to play with:

- network architecture
- learning rate, its decay schedule, update type
- regularization (L2/Dropout strength)

neural networks practitioner
music = loss function

Cross-validation "command center"



Track ratio of weight update / weight magnitude

```
# assume parameter vector W and its gradient vector dW
param_scale = np.linalg.norm(W.ravel())
update = -learning_rate*dW # simple SGD update
update_scale = np.linalg.norm(update.ravel())
W += update # the actual update
print update_scale / param_scale # want ~1e-3
```

ratio between the updates and values: ~ 0.0002 / 0.02 = 0.01 (about okay)
want this to be somewhere around 0.001 or so

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Model Ensembles

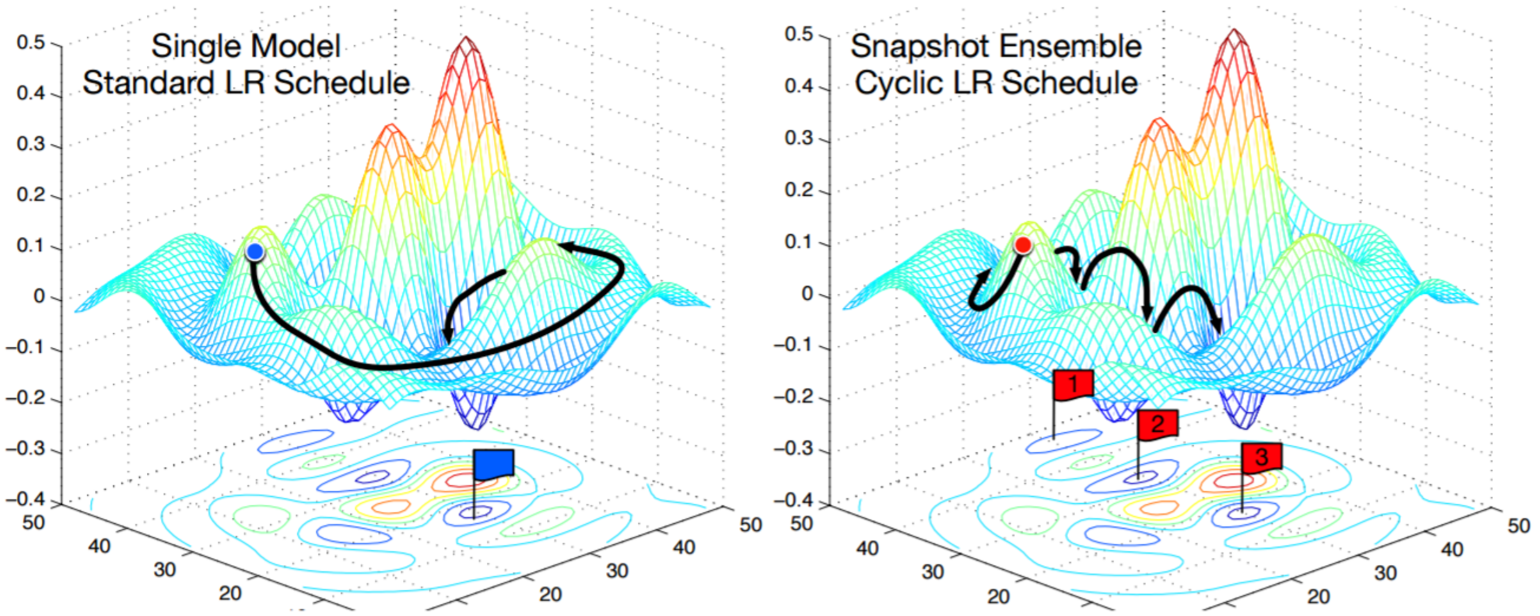
1. Train multiple independent models
2. At test time average their results

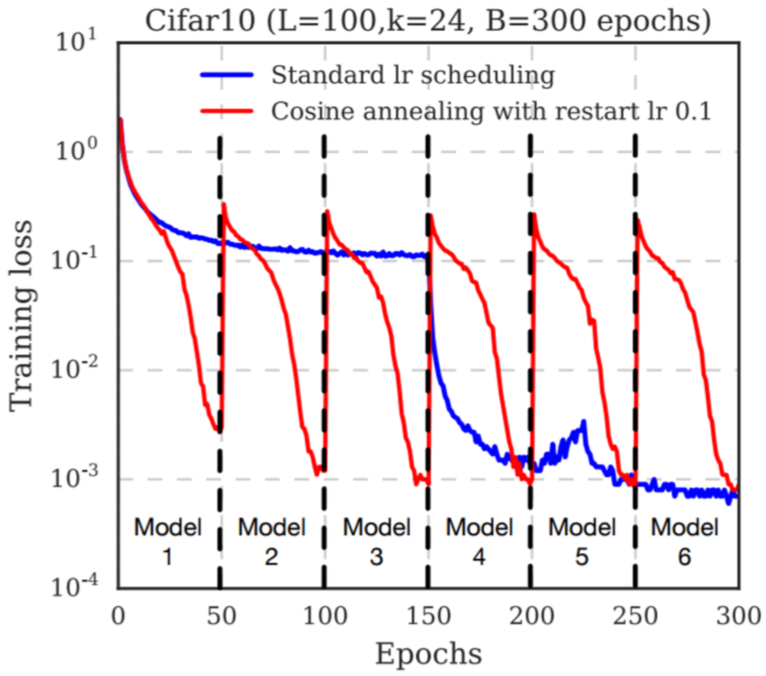
   (Take average of predicted probability distributions, then choose argmax)

Enjoy 2% extra performance

Model Ensembles: Tips and Tricks

Instead of training independent models, use multiple snapshots of a single model during training!





Cyclic learning rate schedules can make this work even better!

Loshchilov and Hutter, “SGDR: Stochastic gradient descent with restarts”, arXiv 2016
Huang et al, “Snapshot ensembles: train 1, get M for free”, ICLR 2017

Model Ensembles: Tips and Tricks

Instead of using actual parameter vector, keep a moving average of the parameter vector and use that at test time (Polyak averaging)

```
while True:
  data_batch = dataset.sample_data_batch()
  loss = network.forward(data_batch)
  dx = network.backward()
  x += - learning_rate * dx
  x_test = 0.995*x_test + 0.005*x # use for test set
```

Polyak and Juditsky, “Acceleration of stochastic approximation by averaging”, SIAM Journal on Control and Optimization, 1992.
Karras et al, “Progressive Growing of GANs for Improved Quality, Stability, and Variation”, ICLR 2018
Brock et al, “Large Scale GAN Training for High Fidelity Natural Image Synthesis”, ICLR 2019

Transfer Learning

Transfer Learning

"You need a lot of a data if you want to train/use CNNs"

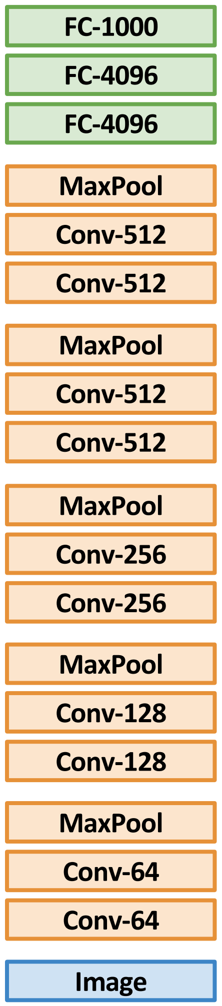
Transfer Learning

"You need a lot of a data if you want to train/use CNNs"

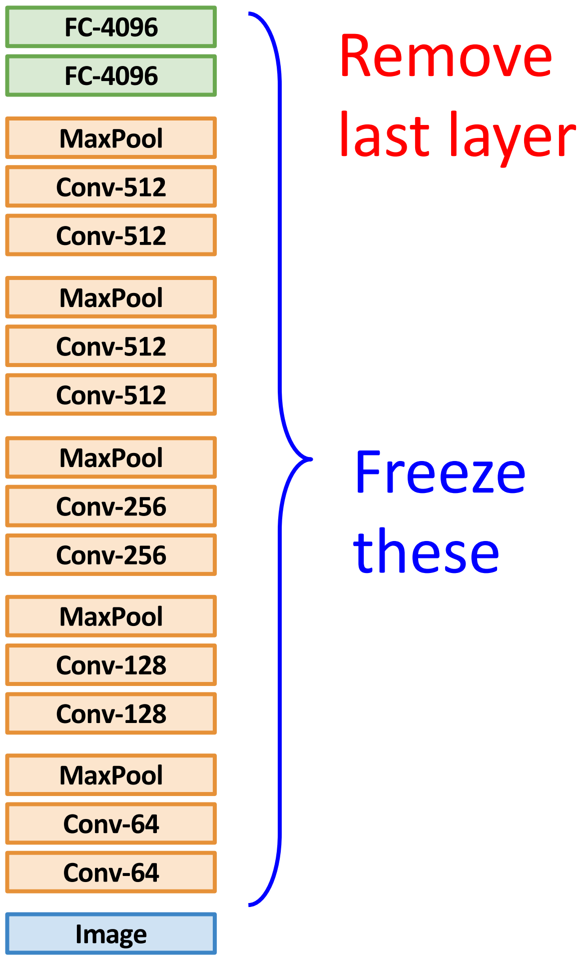
BUSTED

Transfer Learning with CNNs

1. Train on Imagenet



2. Use CNN as a feature extractor



Donahue et al, “DeCAF: A Deep Convolutional Activation Feature for Generic Visual Recognition”, ICML 2014

Transfer Learning with CNNs

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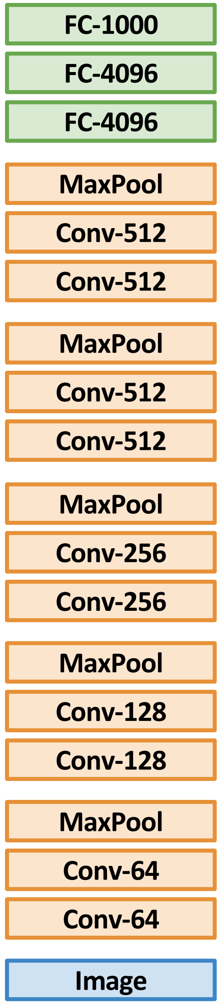
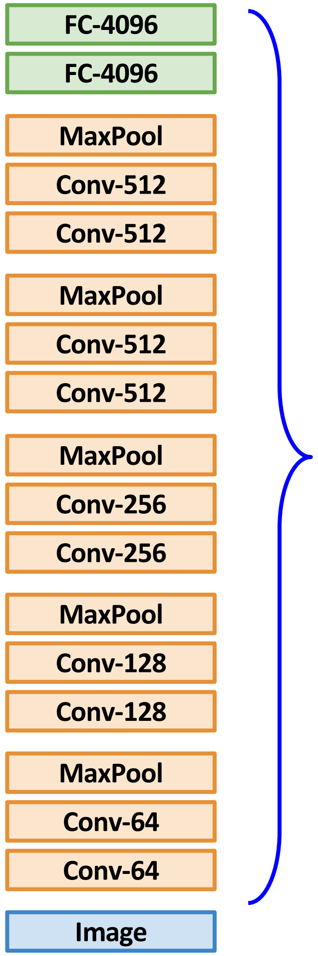


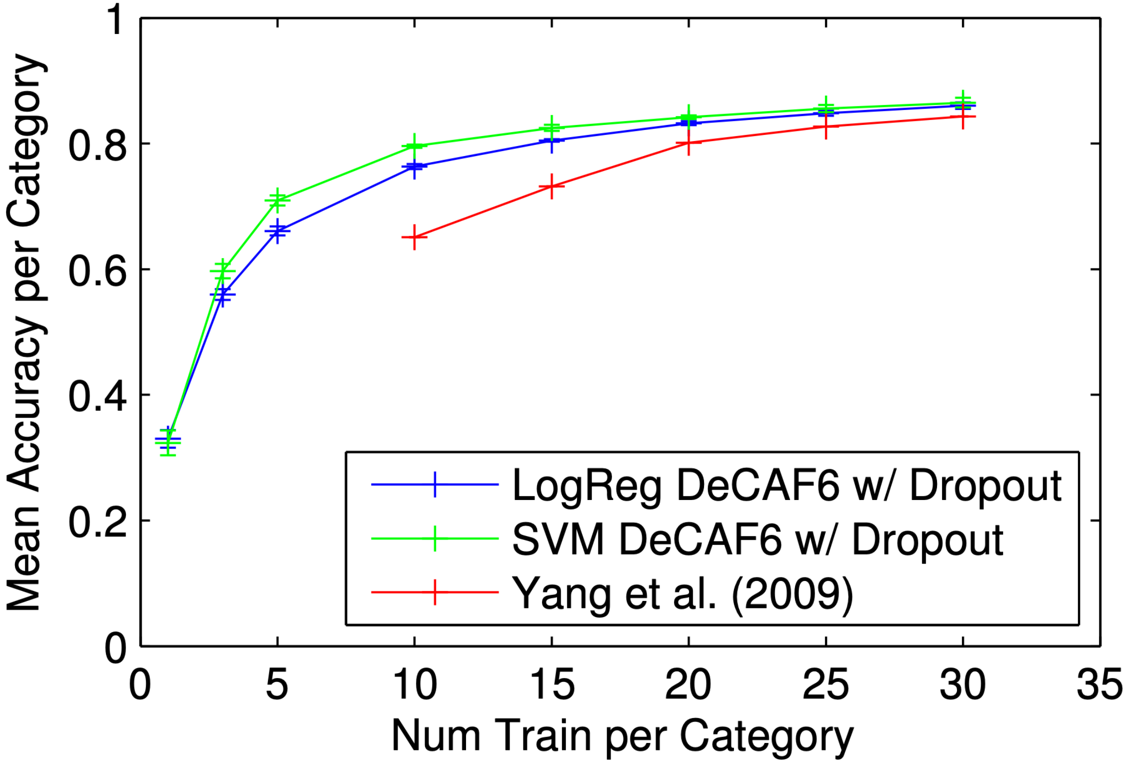
2. Use CNN as a feature extractor



Remove last layer

Freeze these

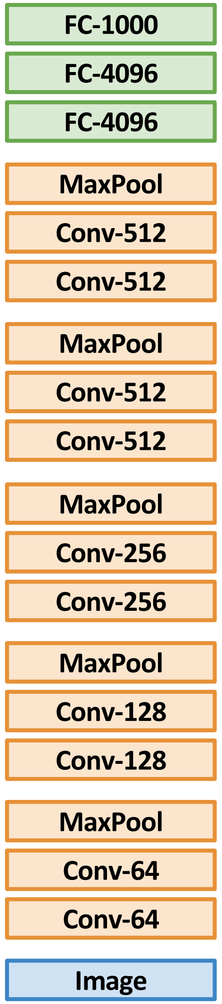
Classification on Caltech-101



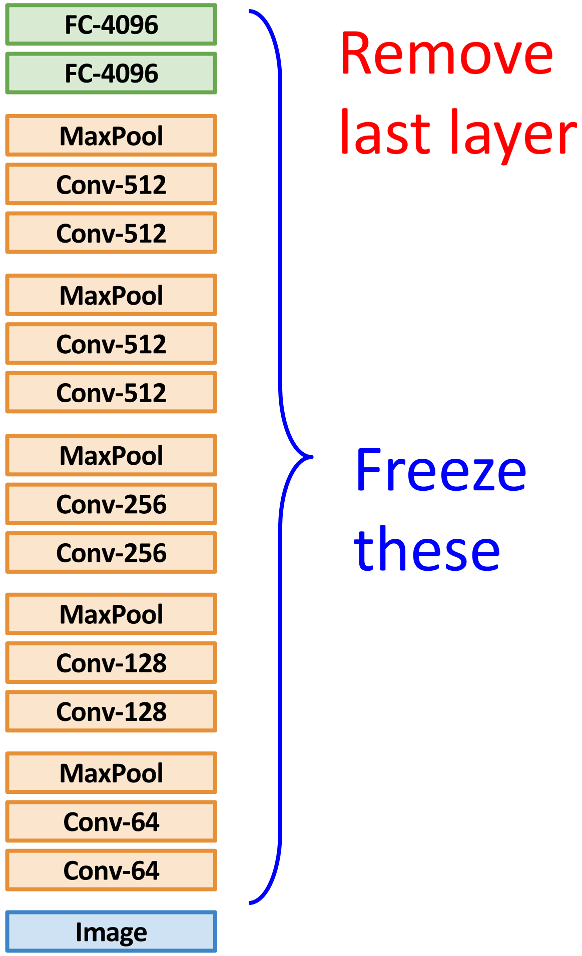
Donahue et al, "DeCAF: A Deep Convolutional Activation Feature for Generic Visual Recognition", ICML 2014

Transfer Learning with CNNs

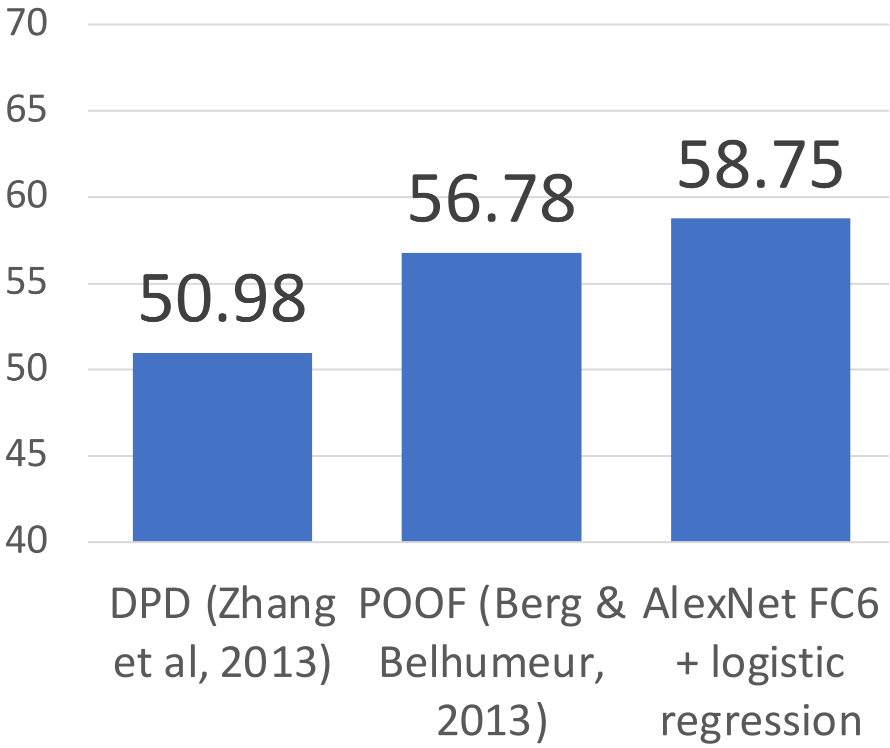
1. Train on Imagenet



2. Use CNN as a feature extractor



Bird Classification on Caltech-UCSD



Donahue et al, “DeCAF: A Deep Convolutional Activation Feature for Generic Visual Recognition”, ICML 2014

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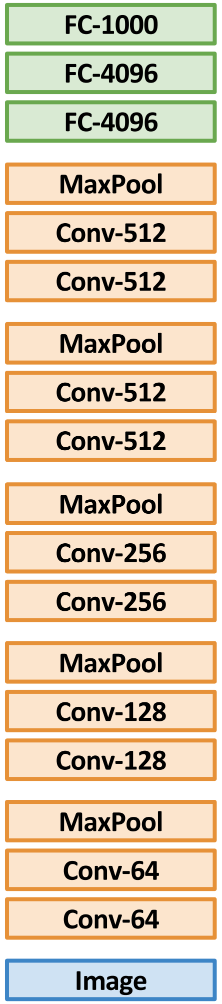

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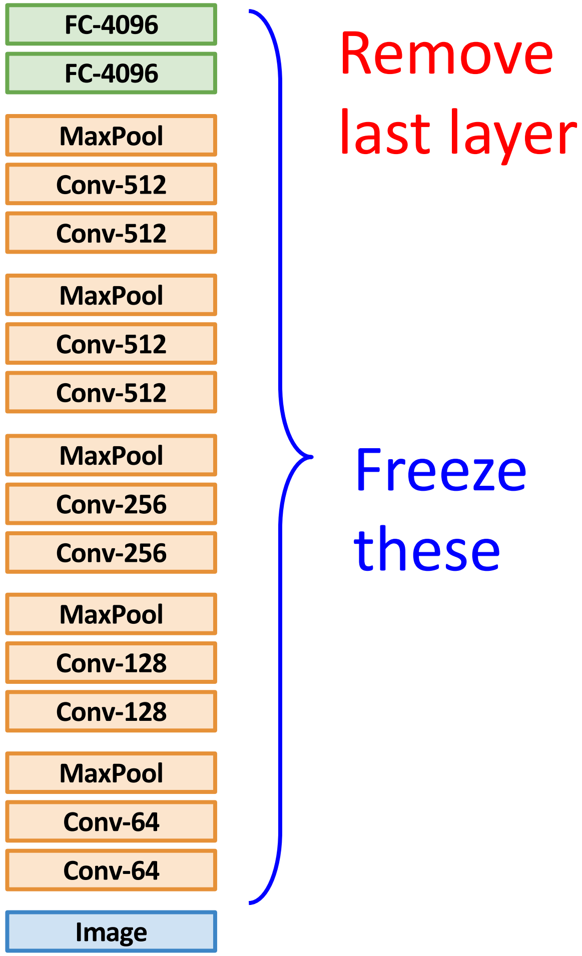

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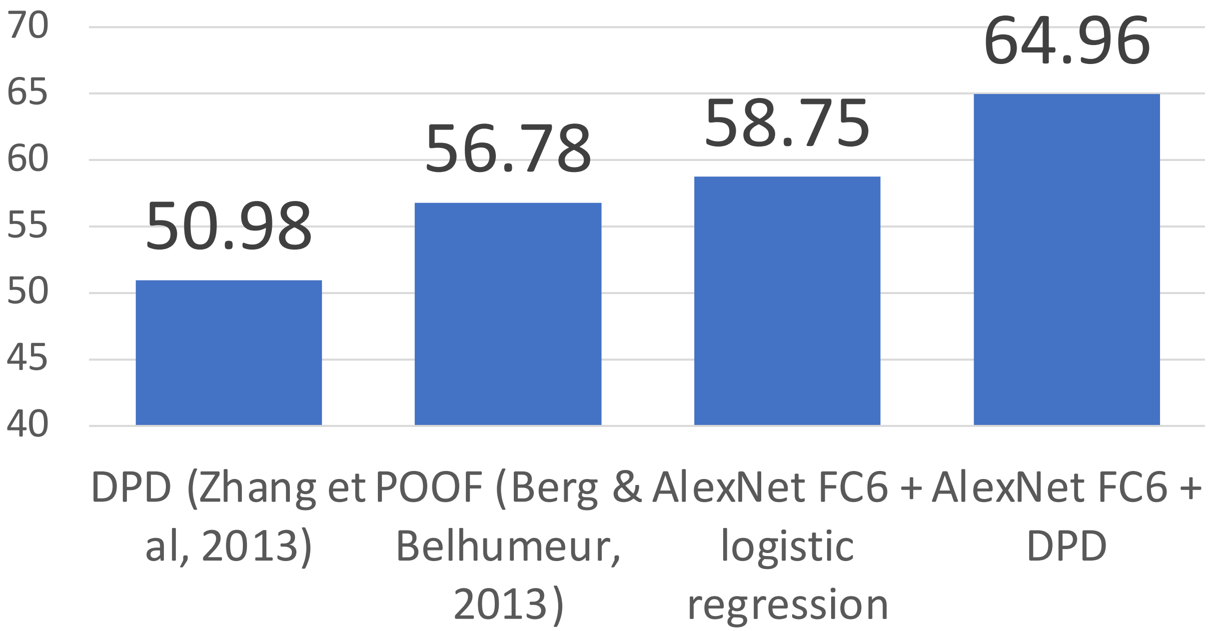

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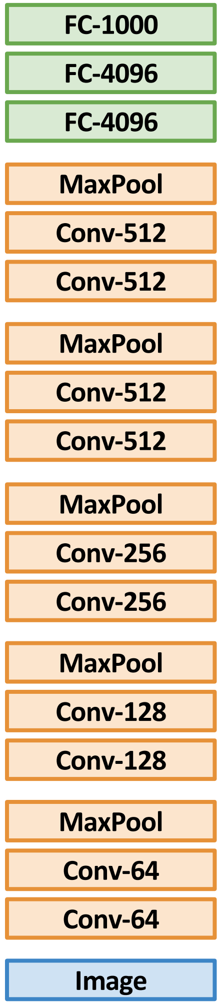

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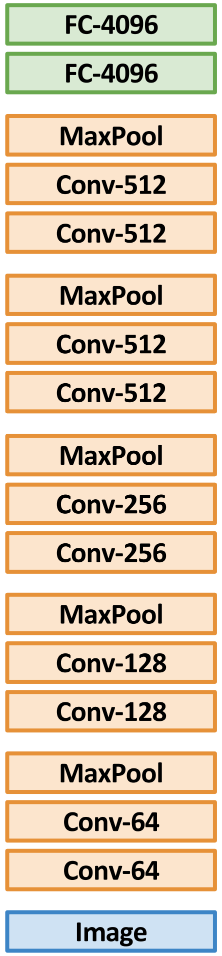

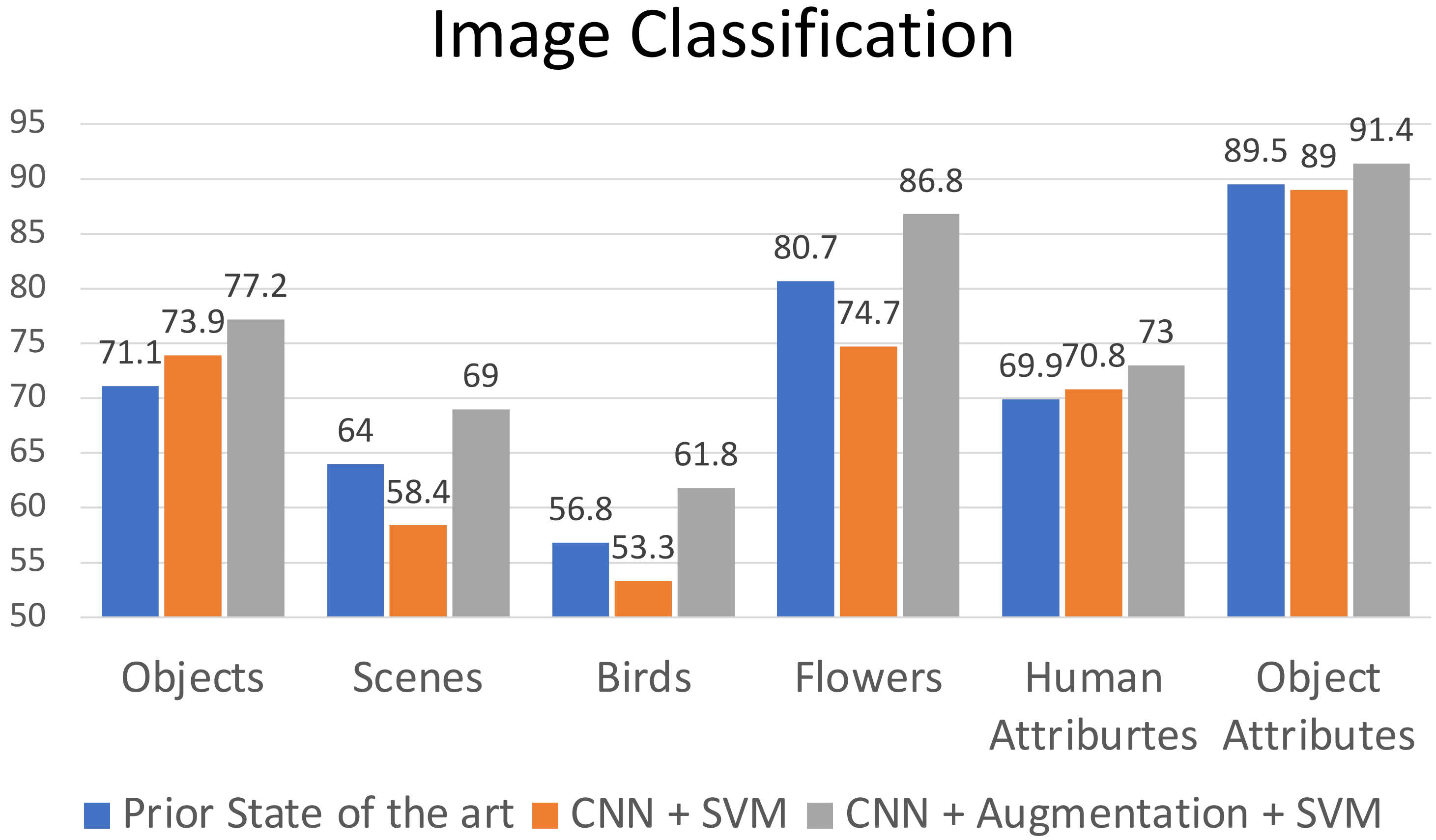

Razavian et al, "CNN Features Off-the-Shelf: An Astounding Baseline for Recognition", CVPR Workshops 2014

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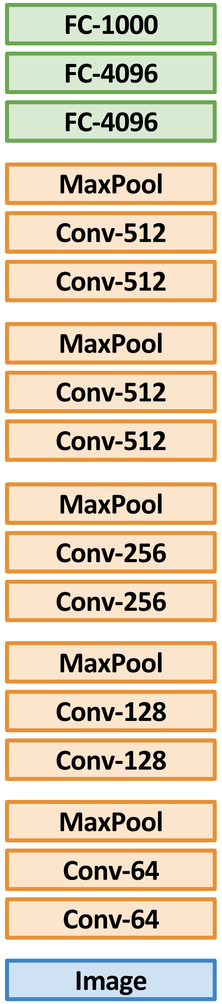

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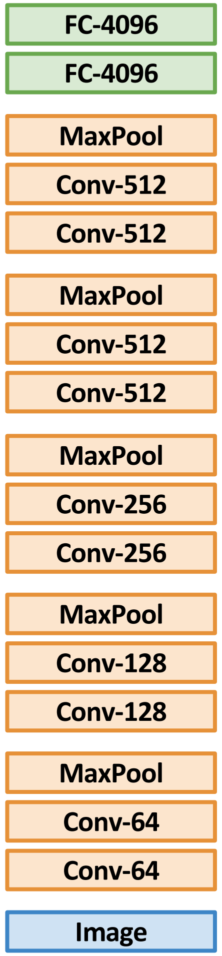
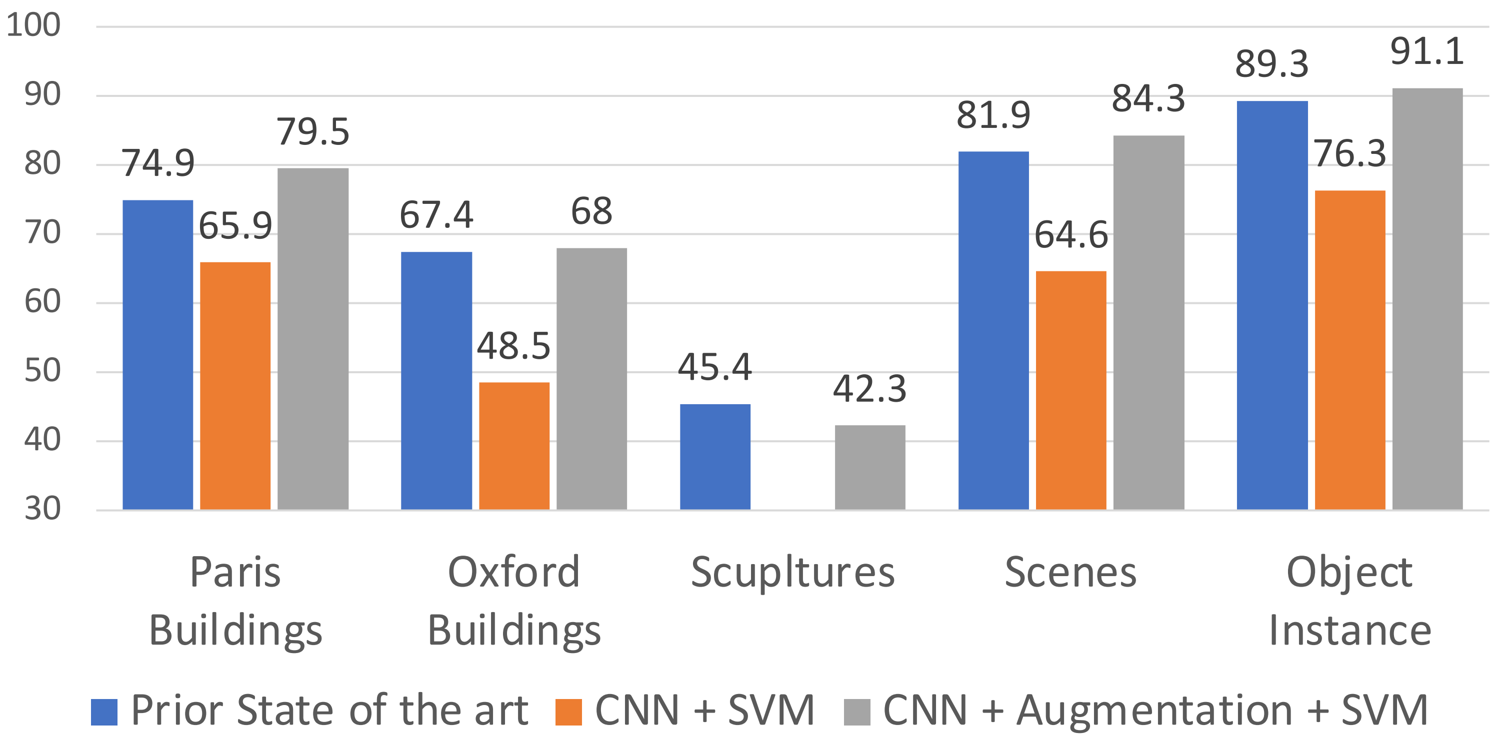


Image Retrieval: Nearest-Neighbor



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Transfer Learning with CNNs

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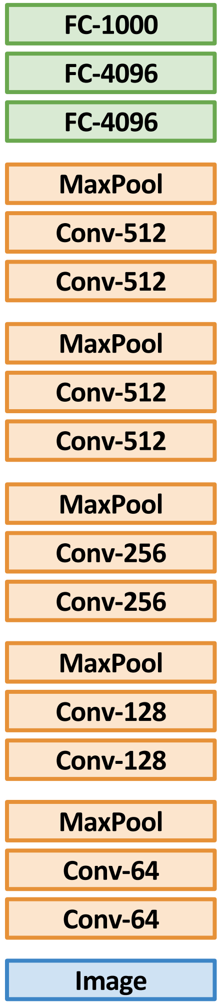

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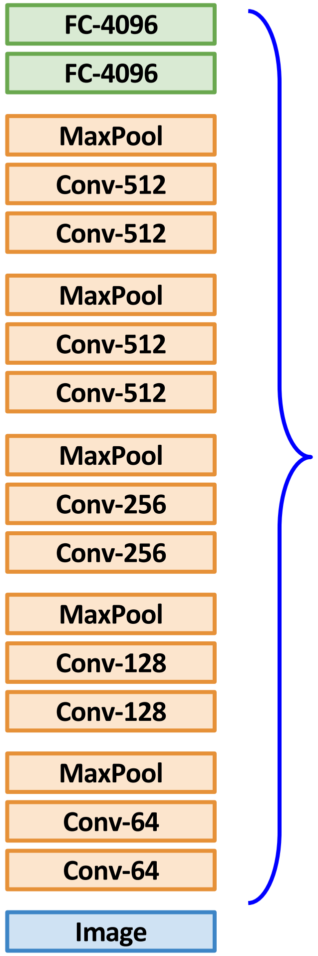
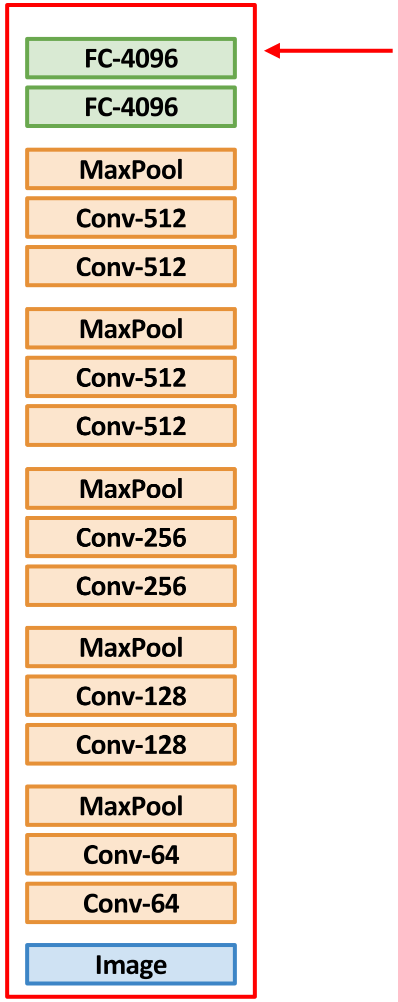


Remove last layer

Freeze these

3. Bigger dataset: **Fine-Tuning**



Continue training CNN for new task!

Transfer Learning with CNNs

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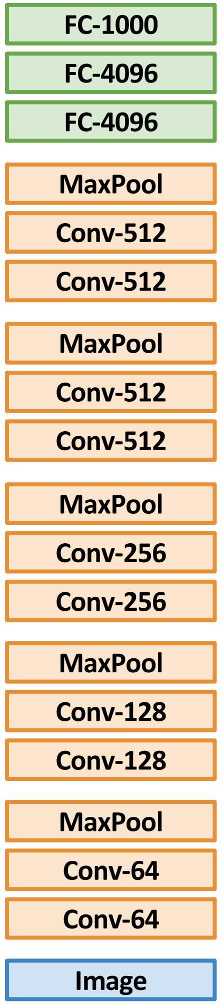

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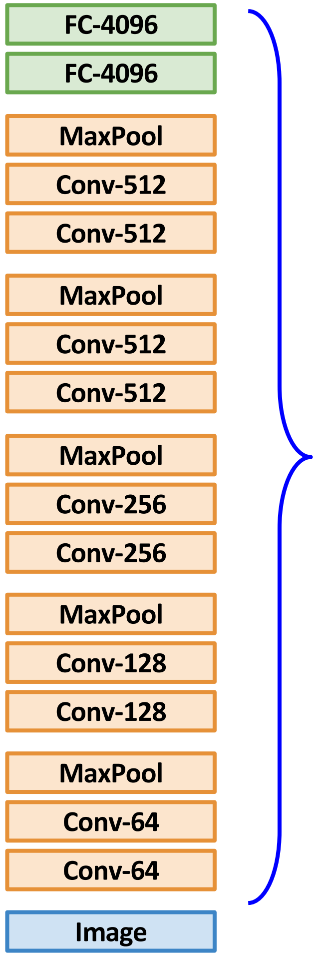

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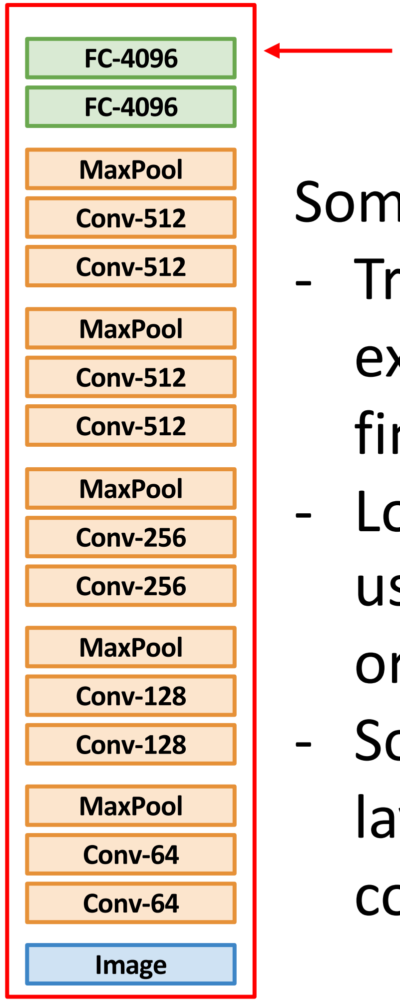

Continue training CNN for new task!

Some tricks:

- Train with feature extraction first before fine-tuning
- Lower the learning rate: use ~1/10 of LR used in original training
- Sometimes freeze lower layers to save computation

Transfer Learning with CNNs

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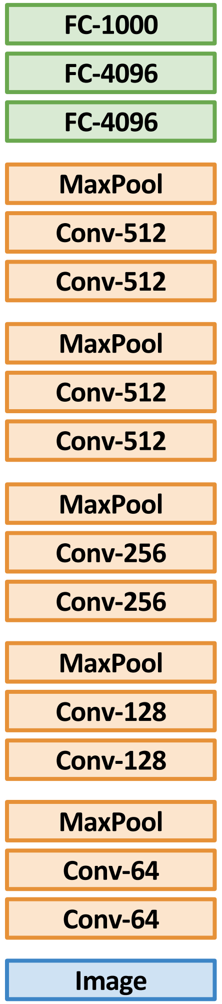

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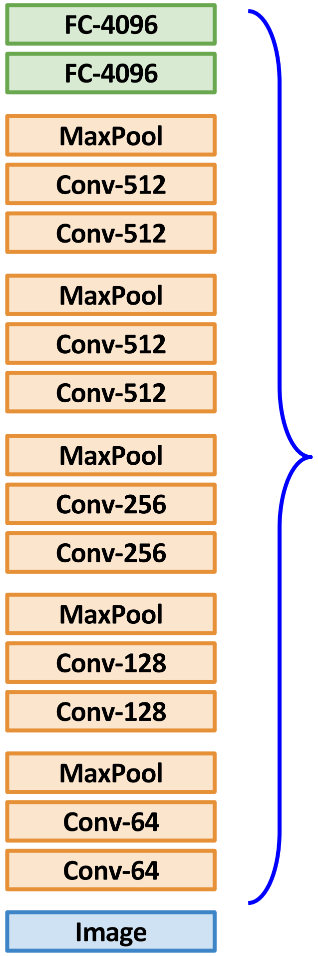

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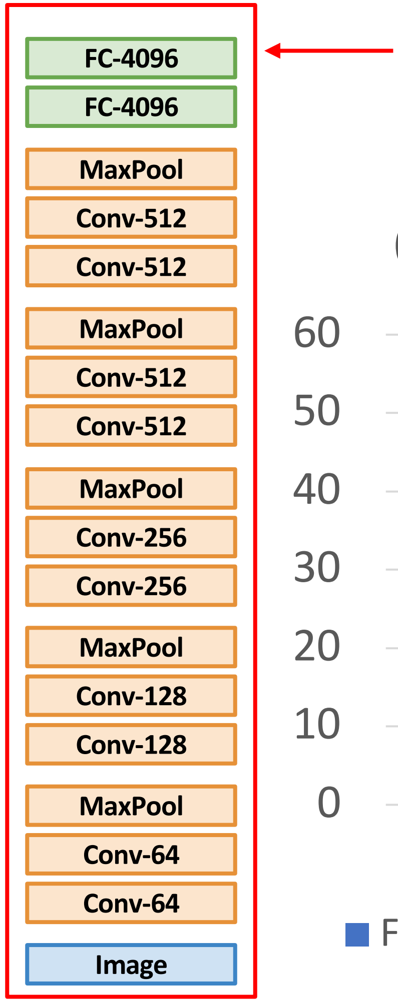
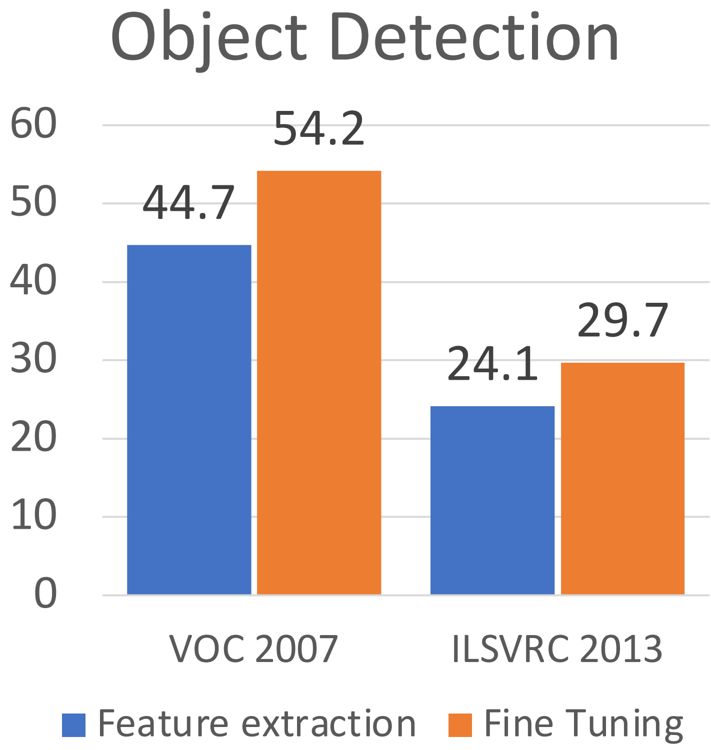
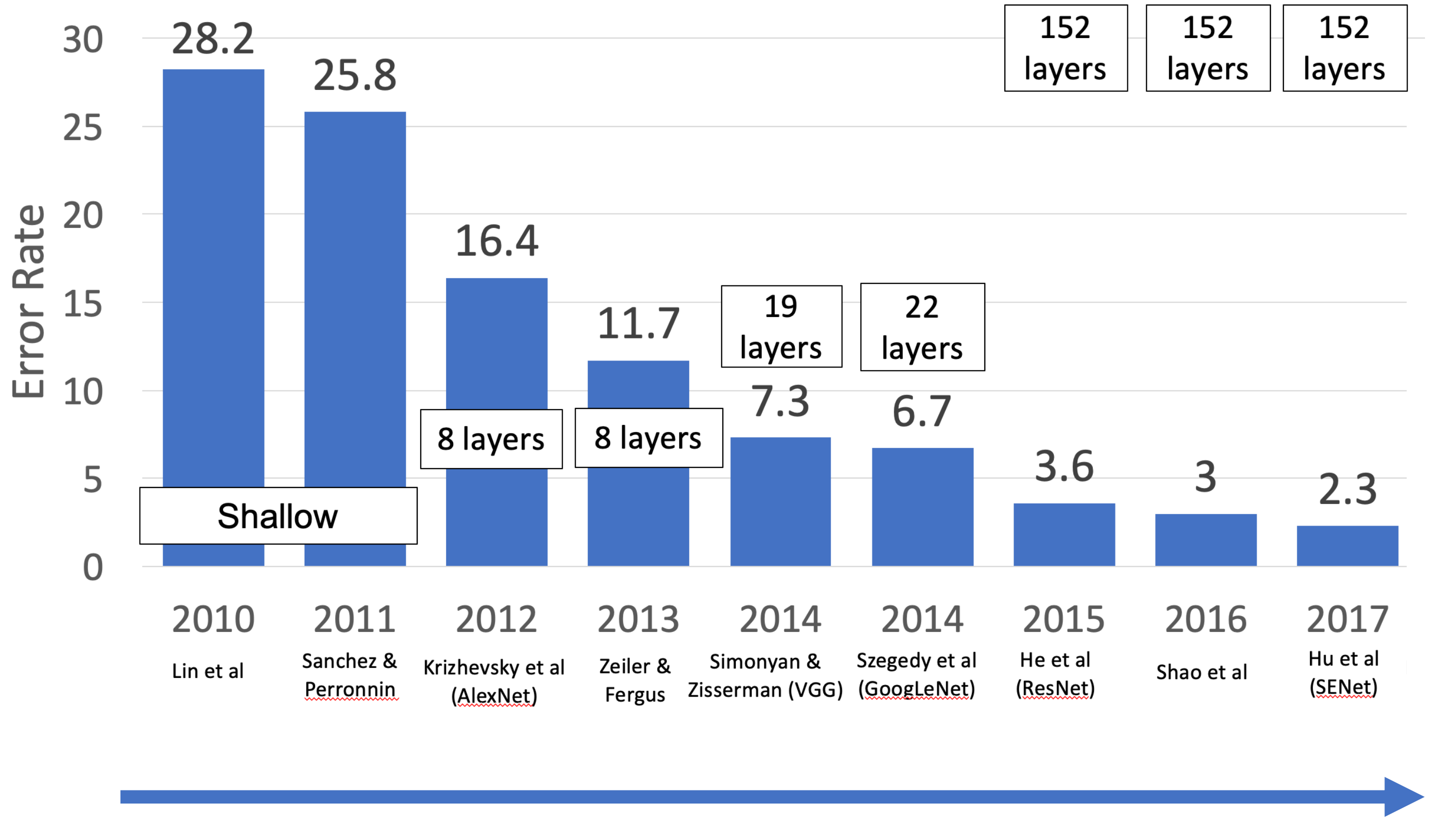


Continue training CNN for new task!



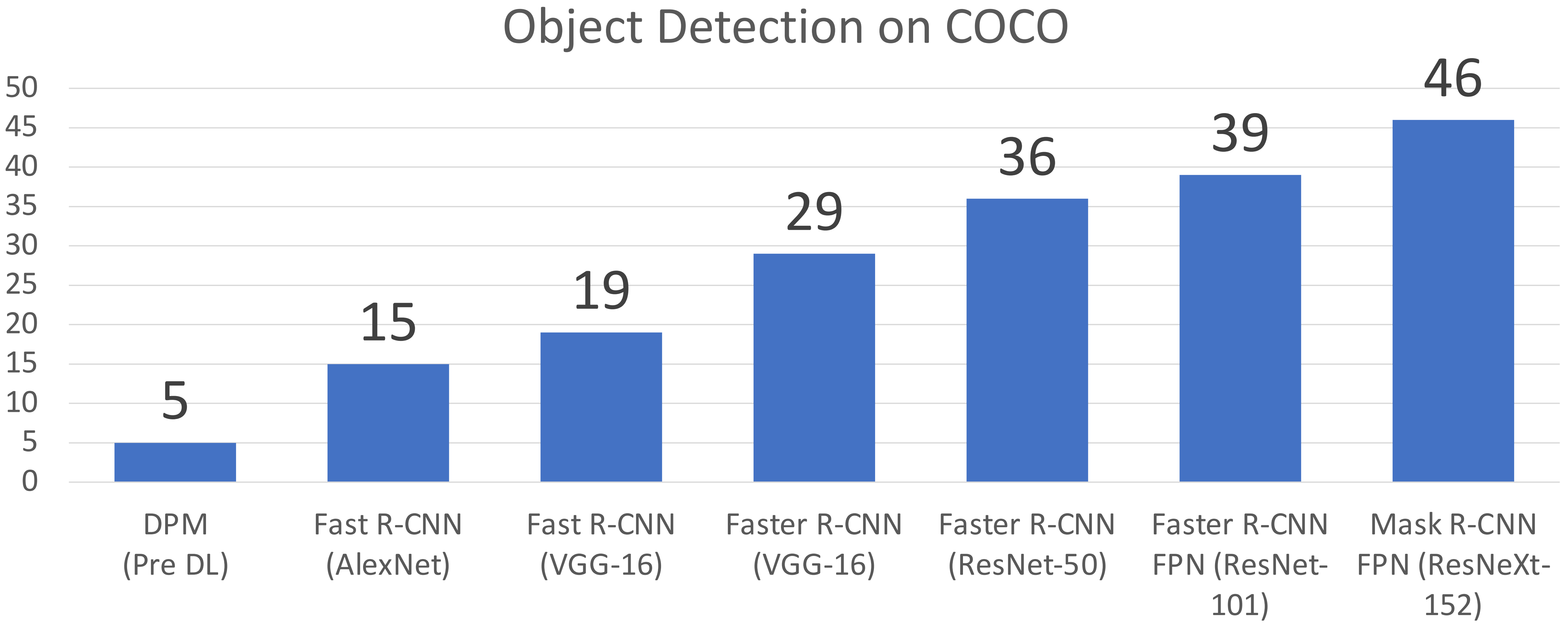
Transfer Learning with CNNs: Architecture Matters!

ImageNet Classification Challenge



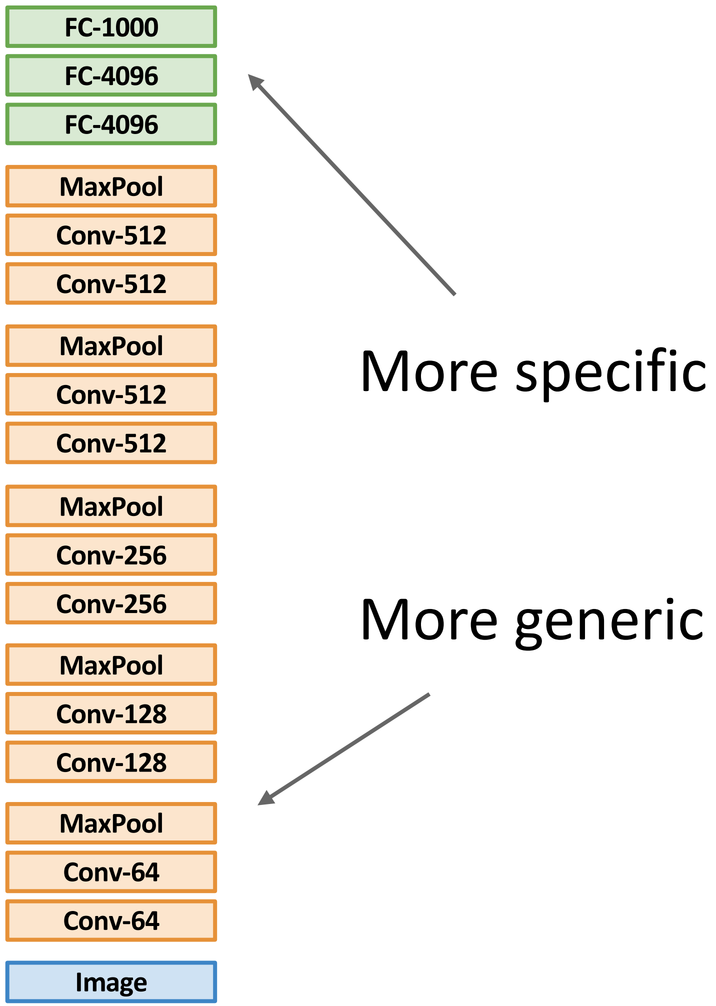
Improvements in CNN architectures lead to improvements in many downstream tasks thanks to transfer learning!

Transfer Learning with CNNs: Architecture Matters!



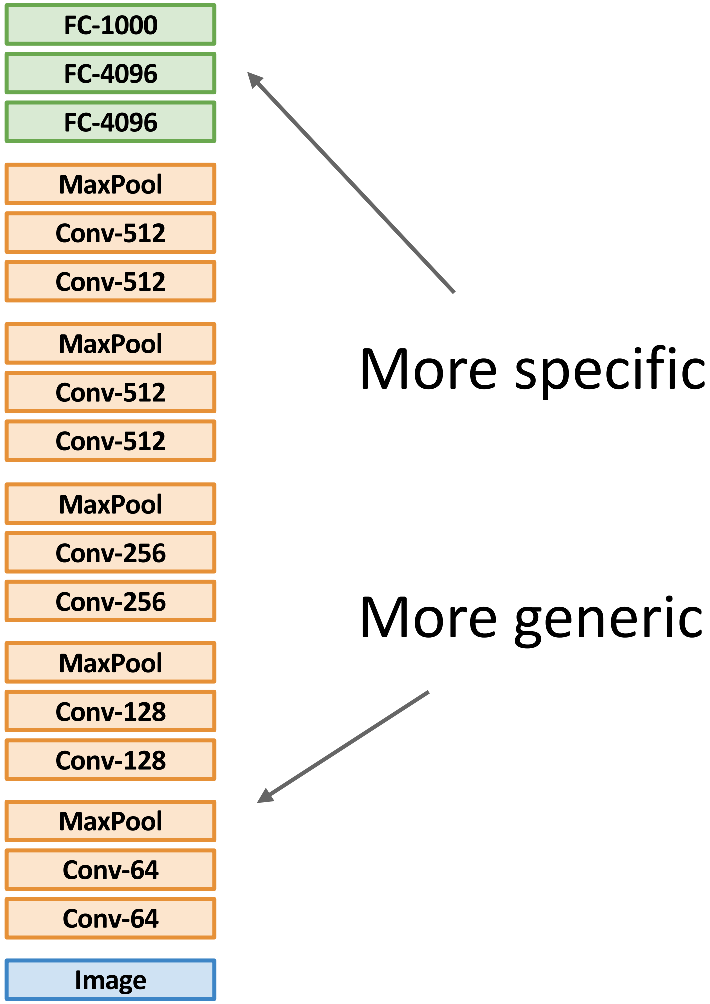
Ross Girshick, “The Generalized R-CNN Framework for Object Detection”, ICCV 2017 Tutorial on Instance-Level Visual Recognition

Transfer Learning with CNNs



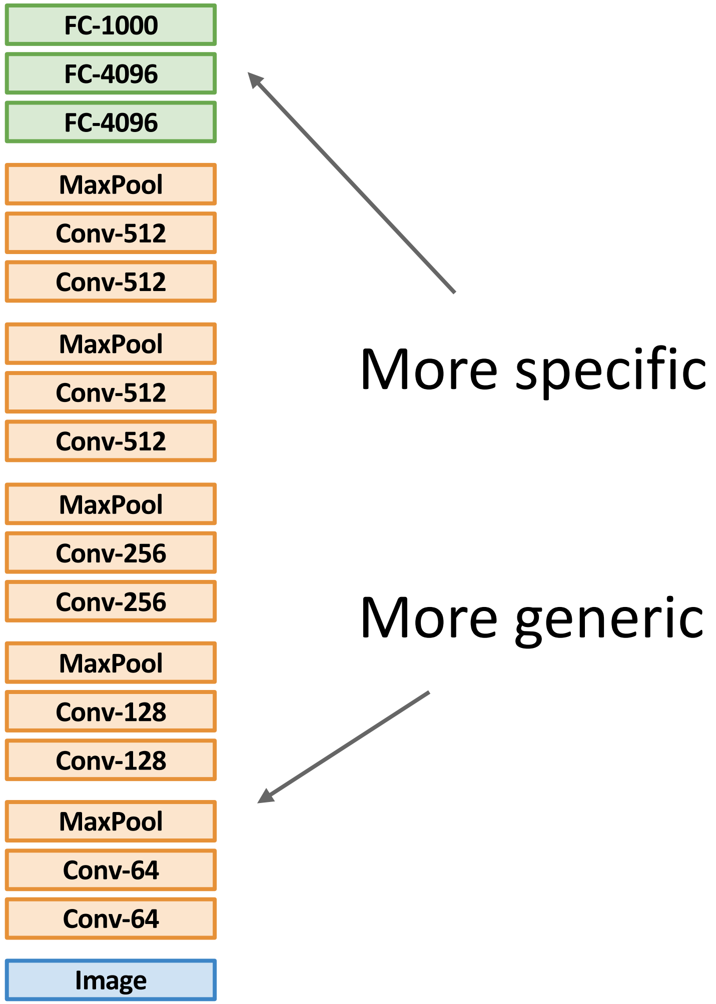
	Dataset similar to ImageNet	Dataset very different from ImageNet
very little data (10s to 100s)	?	?
quite a lot of data (100s to 1000s)	?	?

Transfer Learning with CNNs



	Dataset similar to ImageNet	**Dataset very different from ImageNet**
very little data (10s to 100s)	Use Linear Classifier on top layer	?
quite a lot of data (100s to 1000s)	Finetune a few layers	?

Transfer Learning with CNNs



	Dataset similar to ImageNet	**Dataset very different from ImageNet**
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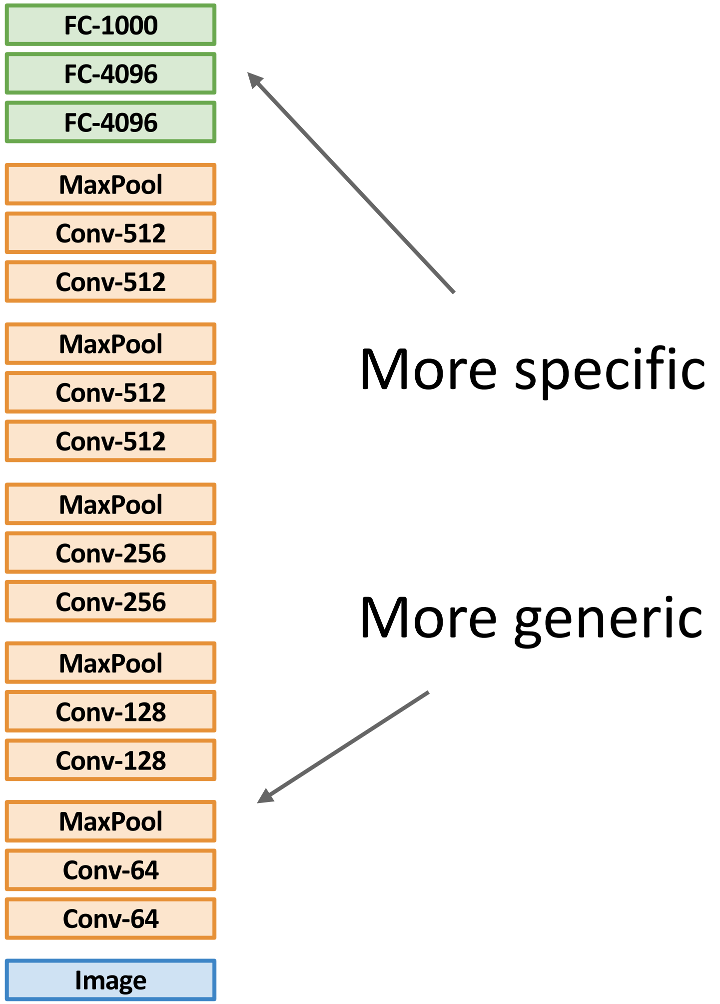
Transfer Learning with CNNs

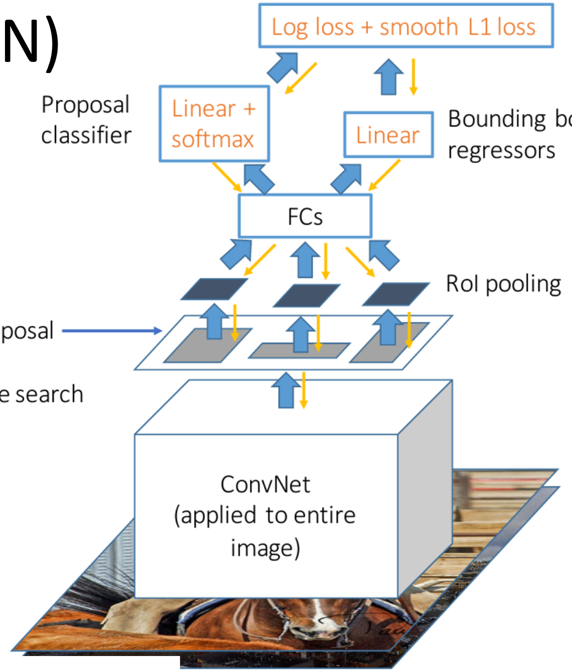


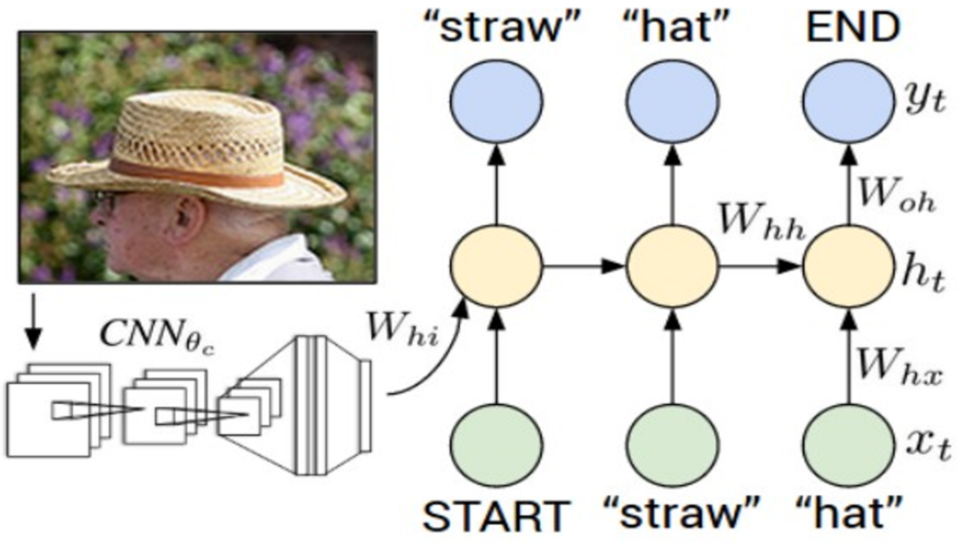
	Dataset similar to ImageNet	**Dataset very different from ImageNet**
very little data (10s to 100s)	Use Linear Classifier on top layer	You're in trouble… Try linear classifier from different stages
quite a lot of data (100s to 1000s)	Finetune a few layers	Finetune a larger number of layers

Transfer learning is pervasive!

It's the norm, not the exception

Object Detection (Fast R-CNN)





Girshick, "Fast R-CNN", ICCV 2015

Karpathy and Fei-Fei, "Deep Visual-Semantic Alignments for Generating Image Descriptions", CVPR 2015

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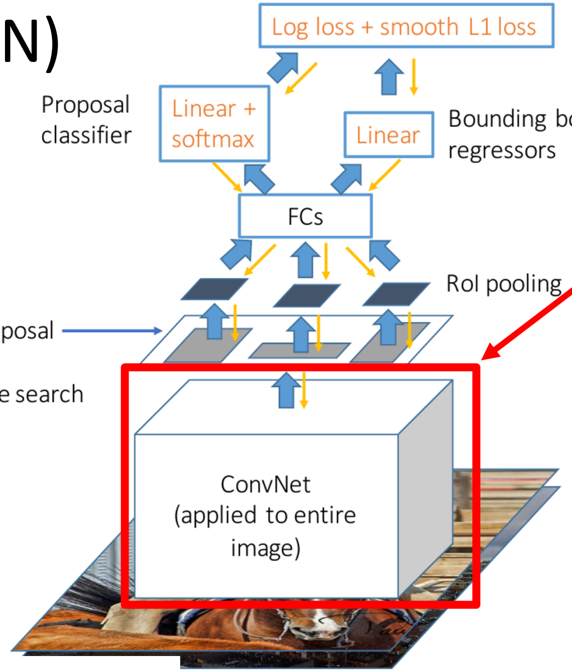
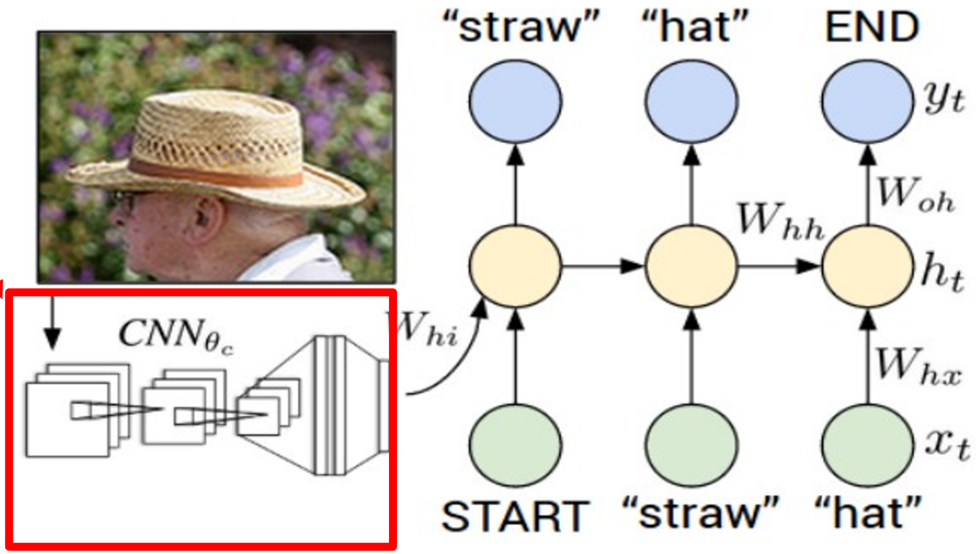


CNN pretrained on ImageNet



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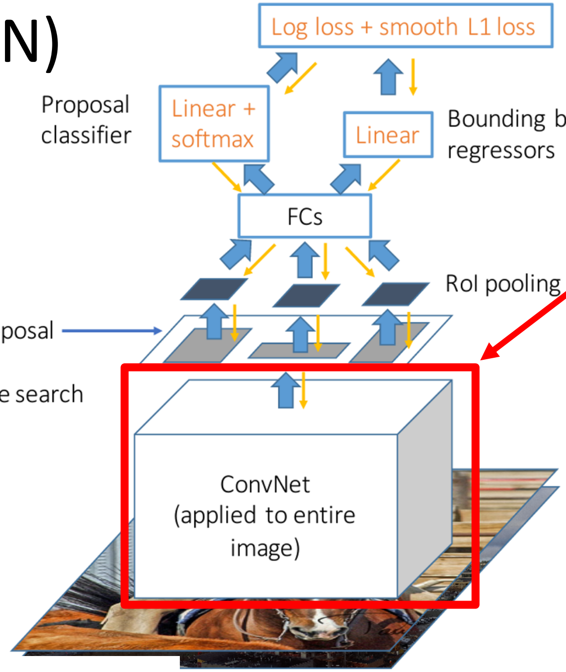
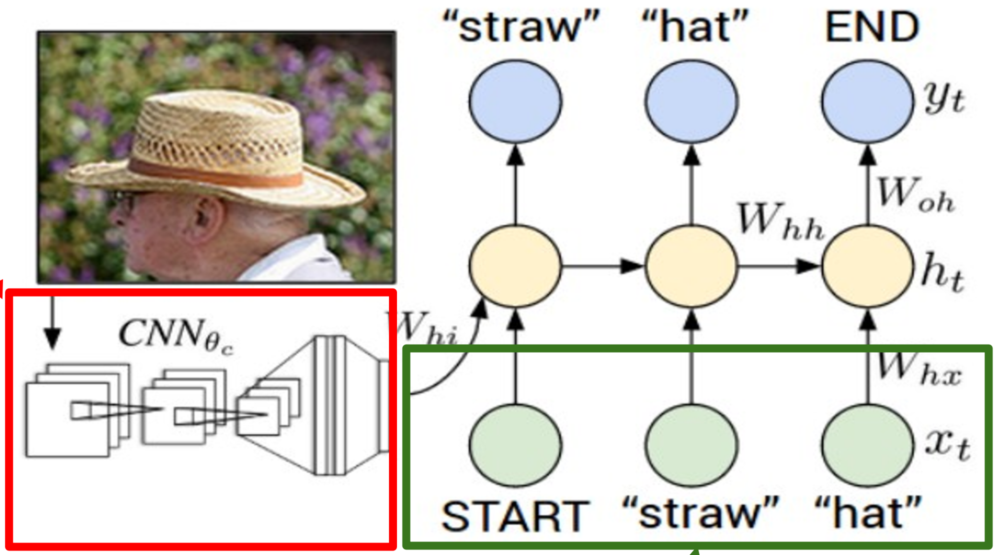


CNN pretrained on ImageNet



Word vectors pretrained with word2vec

Girshick, "Fast R-CNN", ICCV 2015
Figure copyright Ross Girshick, 2015. Reproduced with permission.

Karpathy and Fei-Fei, "Deep Visual-Semantic Alignments for Generating Image Descriptions", CVPR 2015

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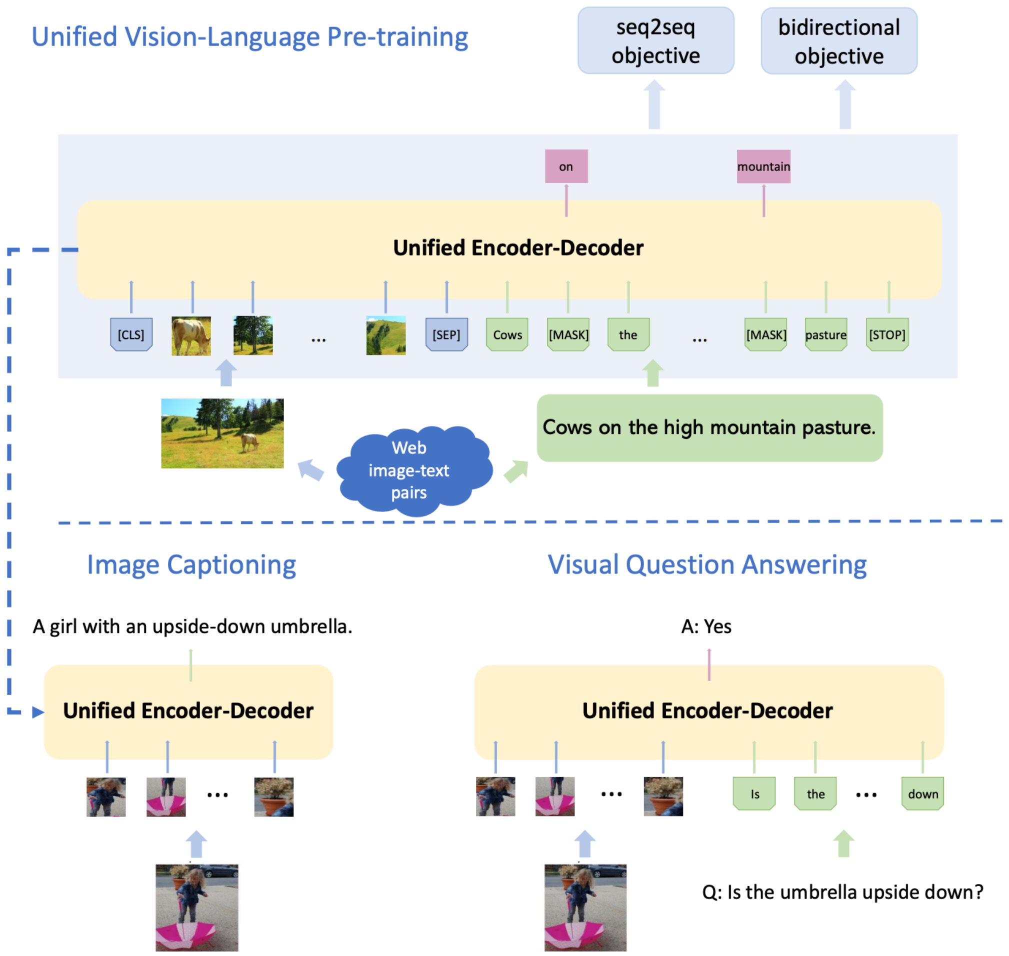


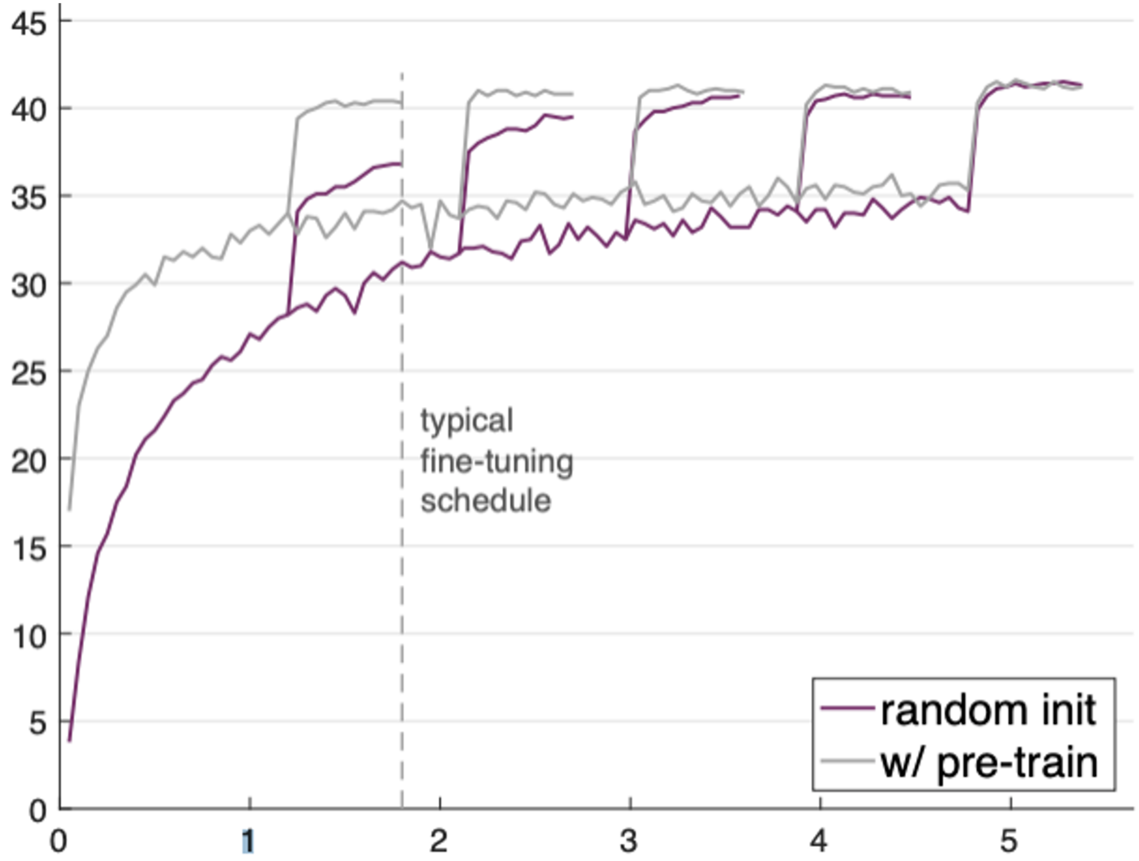
1. Train CNN on ImageNet
2. Fine-Tune (1) for object detection on Visual Genome
3. Train BERT language model on lots of text
4. Combine (2) and (3), train for joint image / language modeling
5. Fine-tune (5) for image captioning, visual question answering, etc.

Zhou et al, "Unified Vision-Language Pre-Training for Image Captioning and VQA", arXiv 2019

Transfer learning is pervasive!

Some very recent results have questioned it

COCO object detection



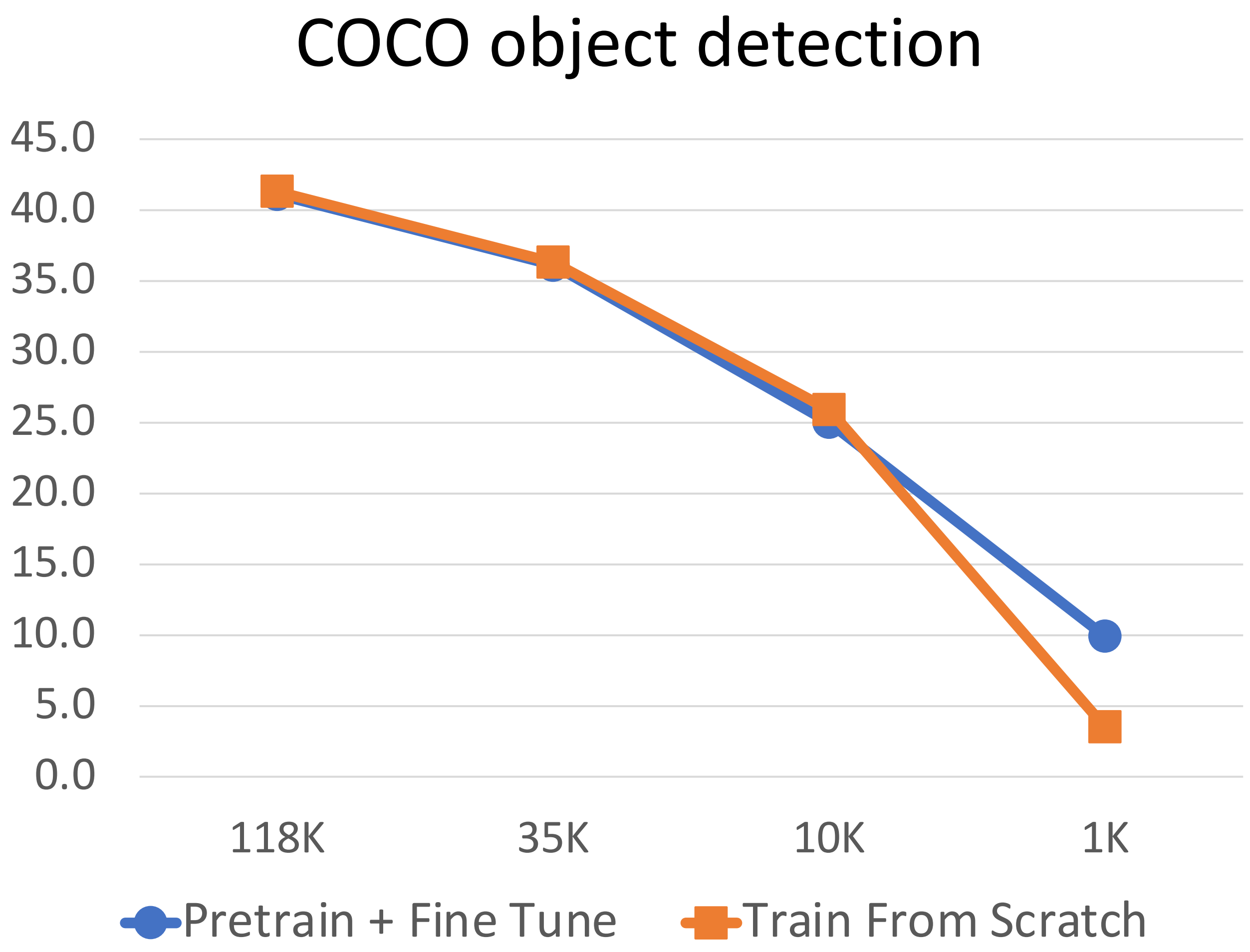
Training from scratch can work as well as pretraining on ImageNet!

… If you train for 3x as long

He et al, "Rethinking ImageNet Pre-Training", ICCV 2019

Transfer learning is pervasive!

Some very recent results have questioned it



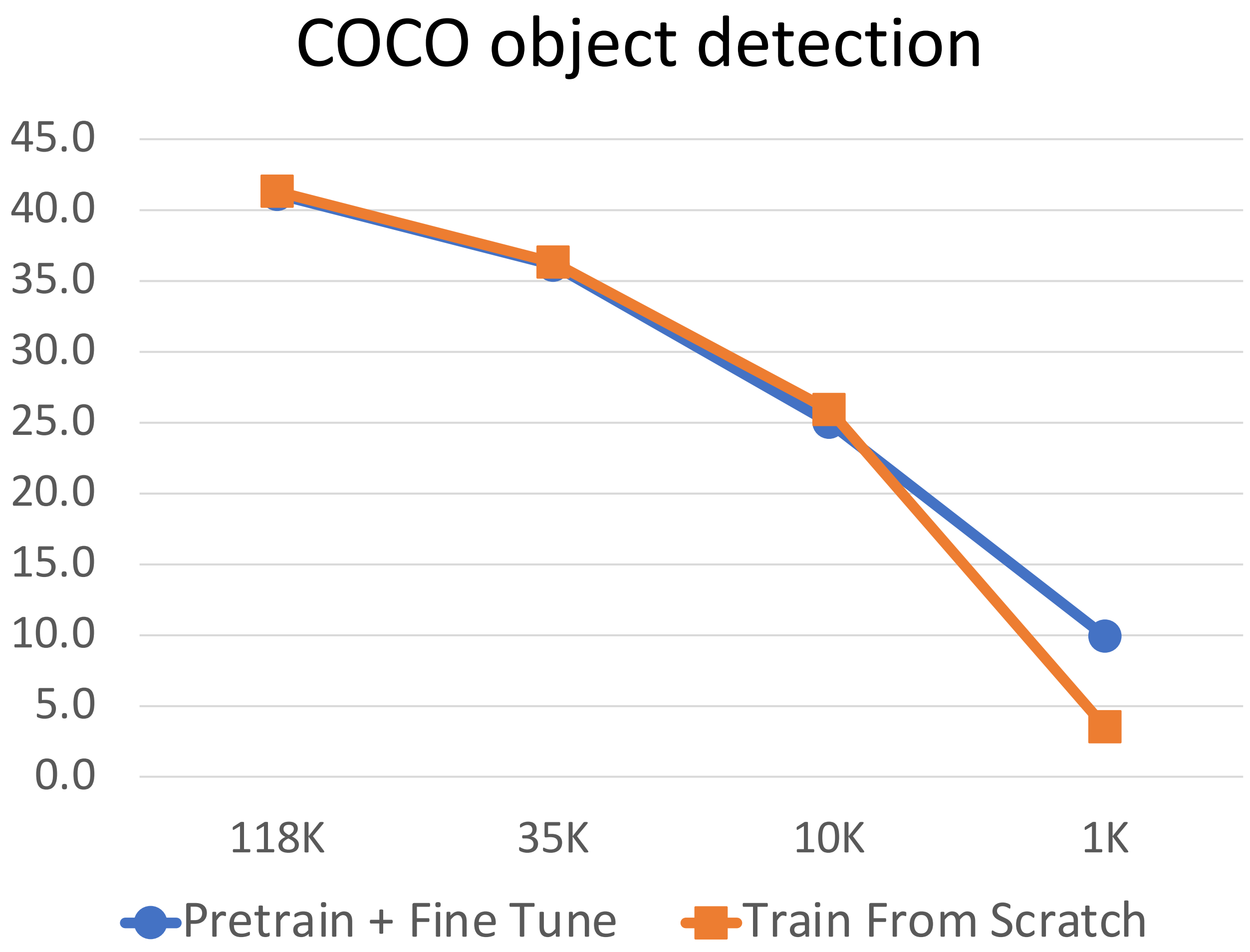
Pretraining + Finetuning beats training from scratch when dataset size is very small

Collecting more data is more effective than pretraining

He et al, "Rethinking ImageNet Pre-Training", ICCV 2019

Transfer learning is pervasive!

Some very recent results have questioned it



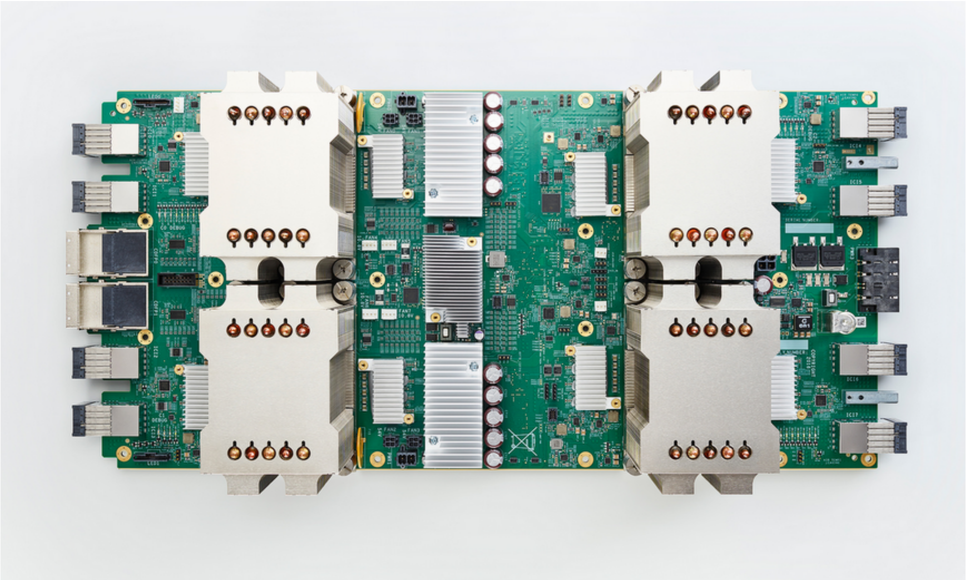
My current view on transfer learning:

- Pretrain+finetune makes your training faster, so practically very useful
- Training from scratch works well once you have enough data
- Lots of work left to be done

He et al, "Rethinking ImageNet Pre-Training", ICCV 2019

Distributed Training

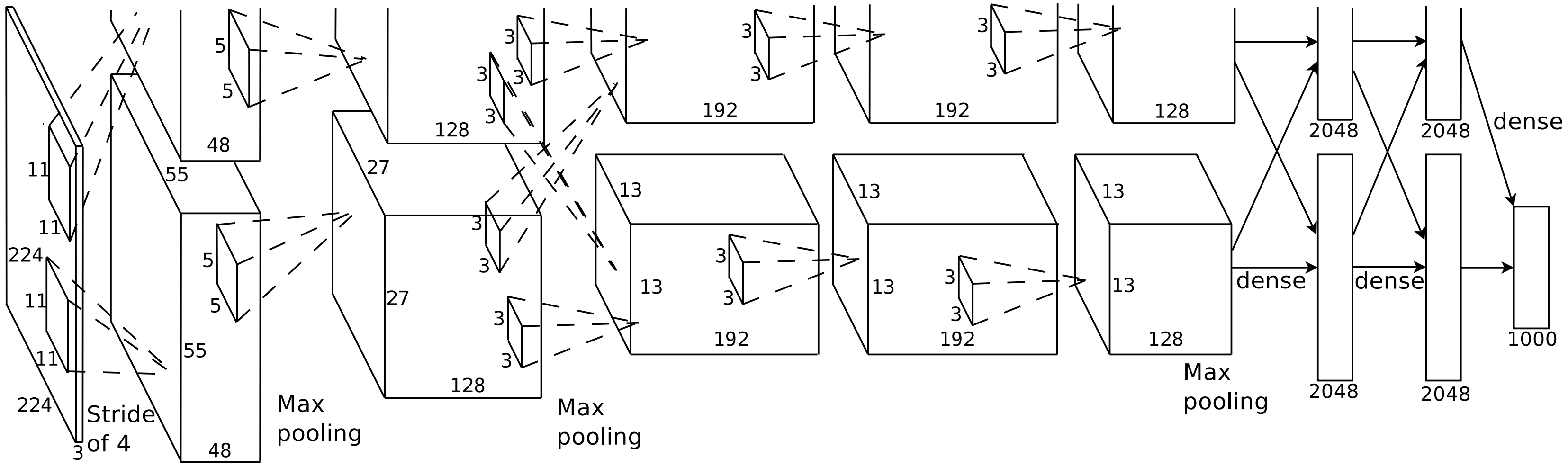
Beyond individual devices



Cloud TPU v2
180 TFLOPs
64 GB HBM memory
$4.50 / hour
(free on Colab!)

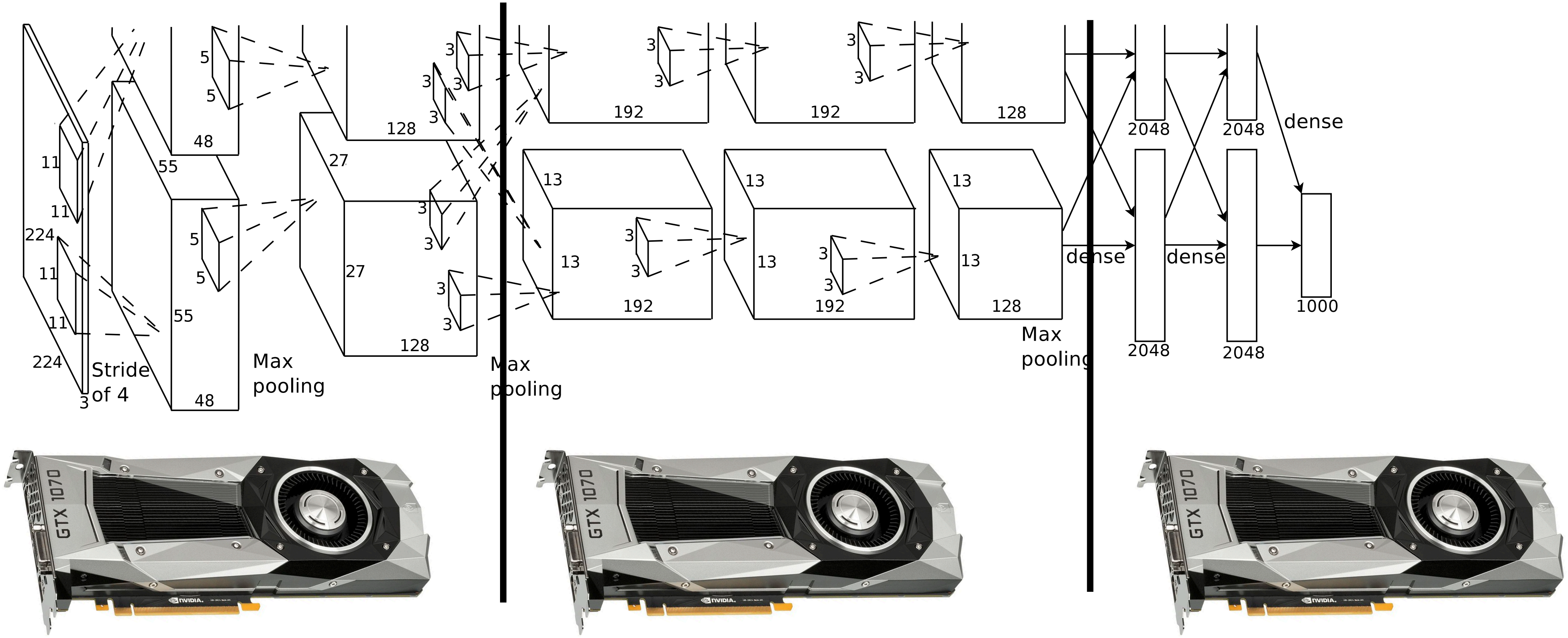
Cloud TPU v2 Pod
64 TPU-v2
11.5 PFLOPs
$384 / hour

Model Parallelism: Split Model Across GPUs



Model Parallelism: Split Model Across GPUs

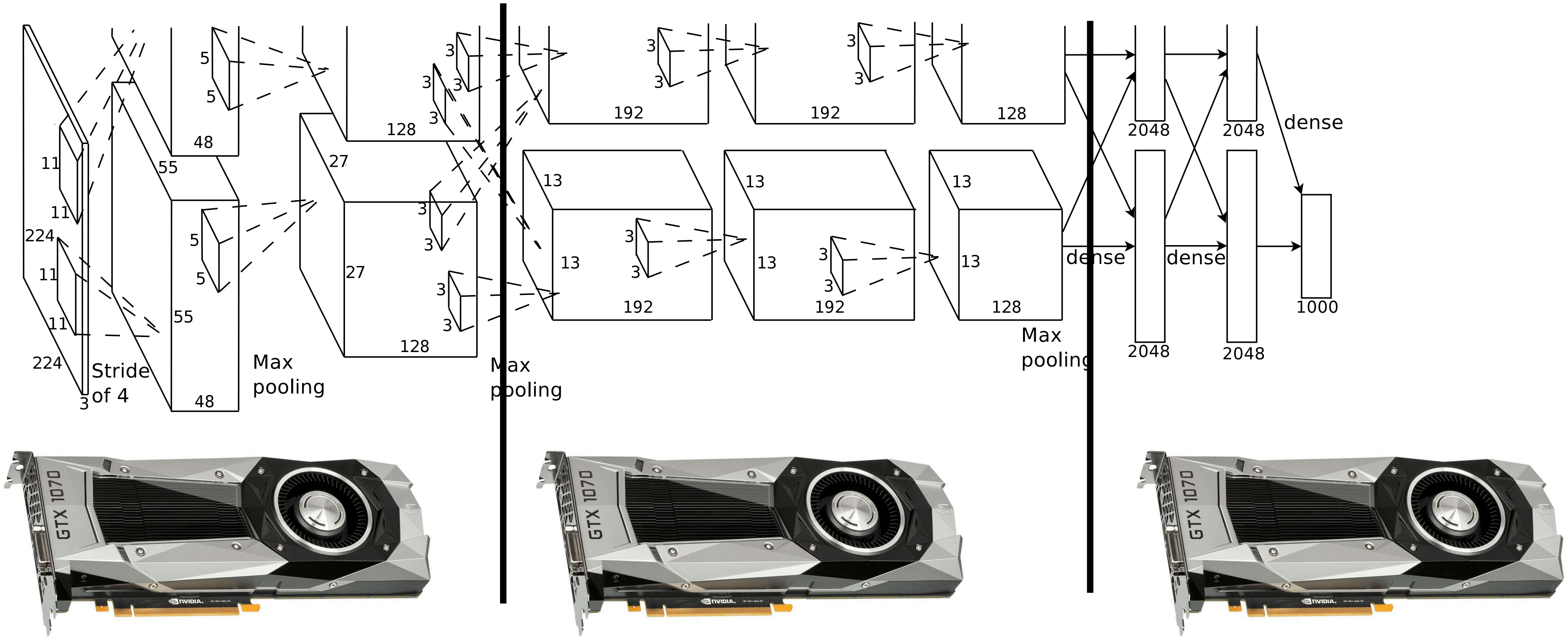
Idea #1: Run different layers on different GPUs



Model Parallelism: Split Model Across GPUs

Idea #1: Run different layers on different GPUs

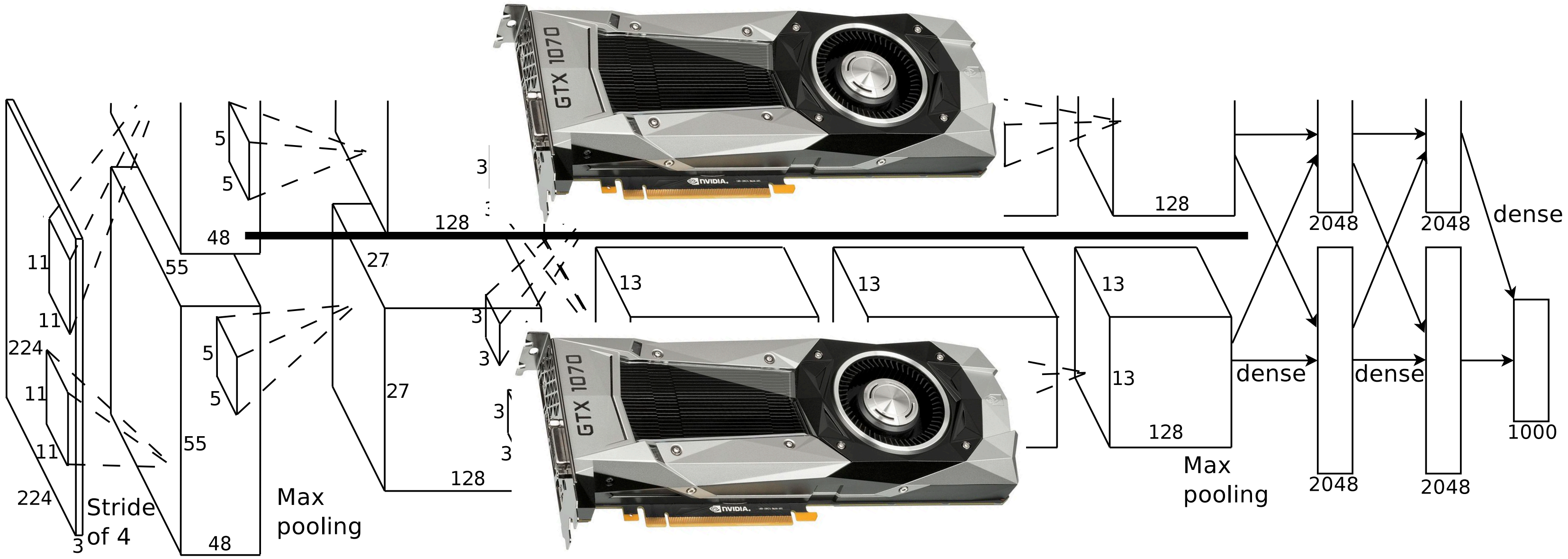
Problem: GPUs spend lots of time waiting



This image is in the public domain

Model Parallelism: Split Model Across GPUs

Idea #2: Run parallel branches of model on different GPUs

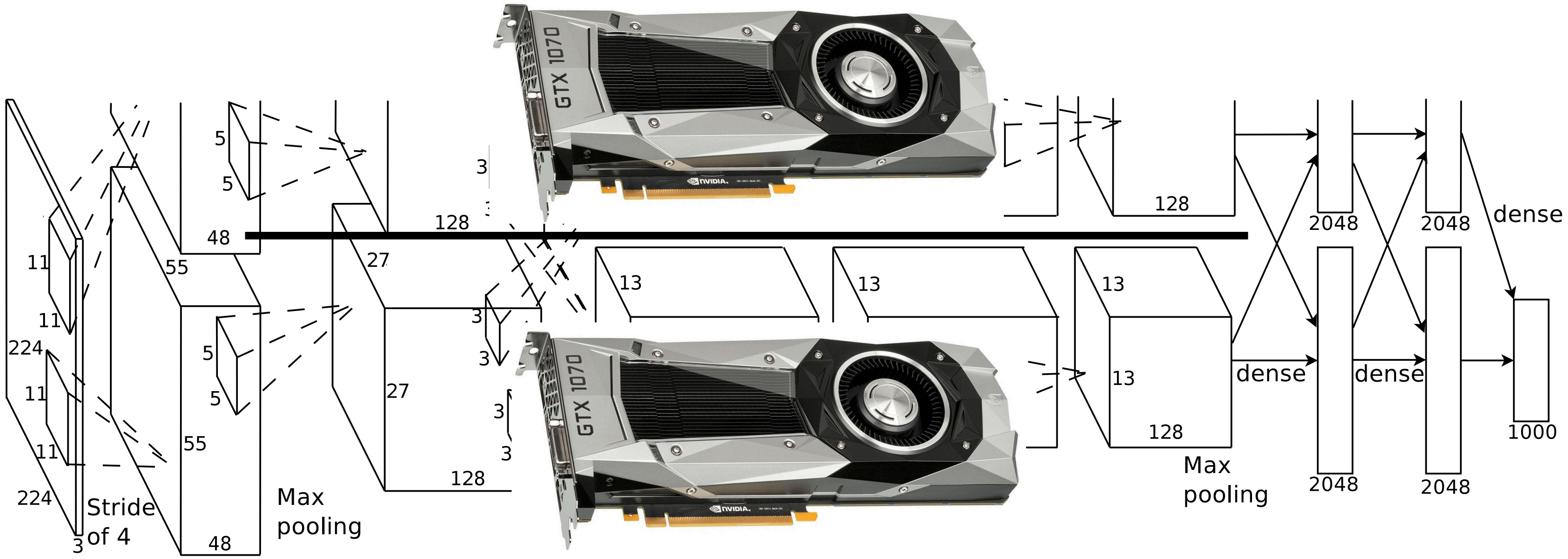


Model Parallelism: Split Model Across GPUs

Idea #2: Run parallel branches of model on different GPUs

Problem: Synchronizing across GPUs is expensive;

Need to communicate **activations** and **grad activations**

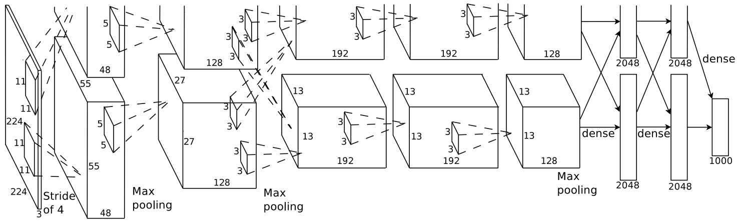


This image is in the public domain

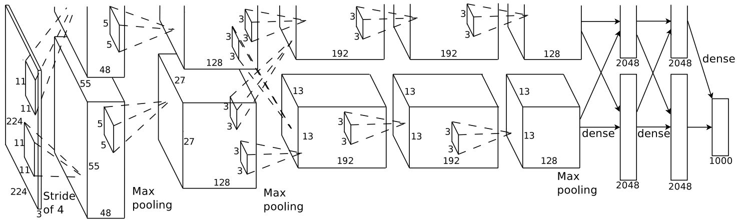
Data Parallelism: Copy Model on each GPU, split data

Batch of
N images

N / 2
images



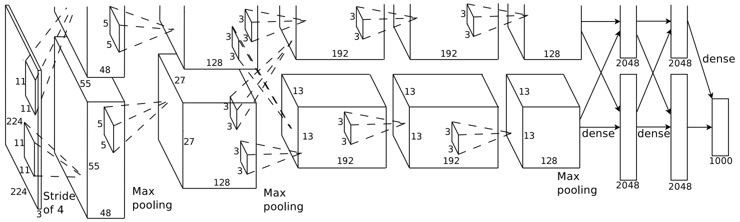
N / 2
images



Data Parallelism: Copy Model on each GPU, split data

Forward: compute loss

N / 2
images



Batch of
N images

Forward: compute loss

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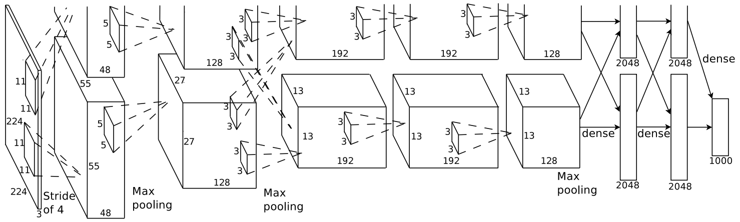

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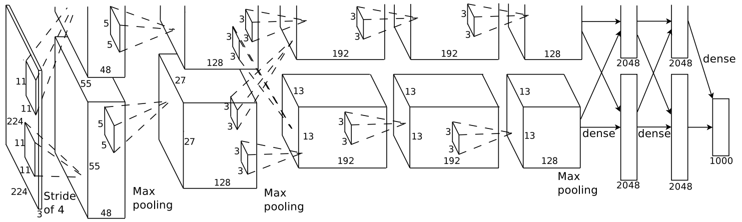
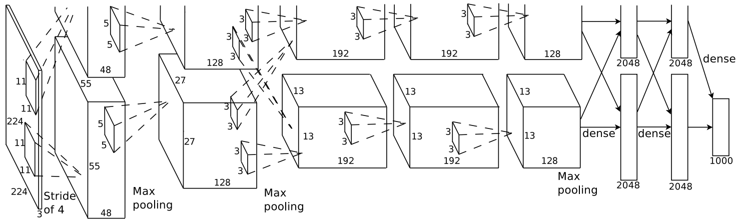


Backward: Compute gradient

Batch of
N images

Forward: compute loss

N / 2
images

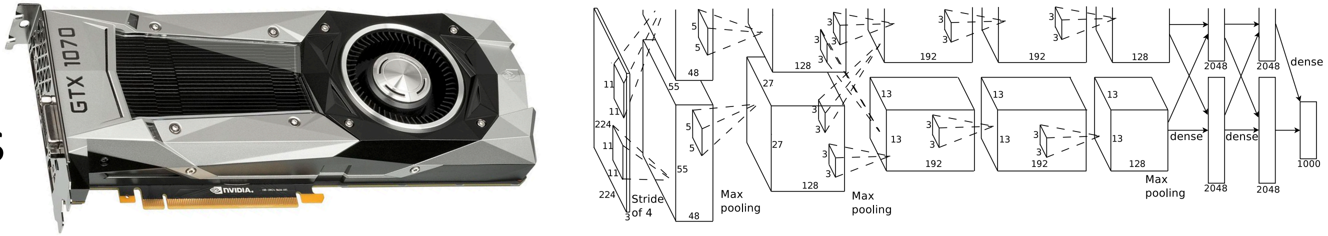


Backward: Compute gradient

Data Parallelism: Copy Model on each GPU, split data

Forward: compute loss

N / 2
images



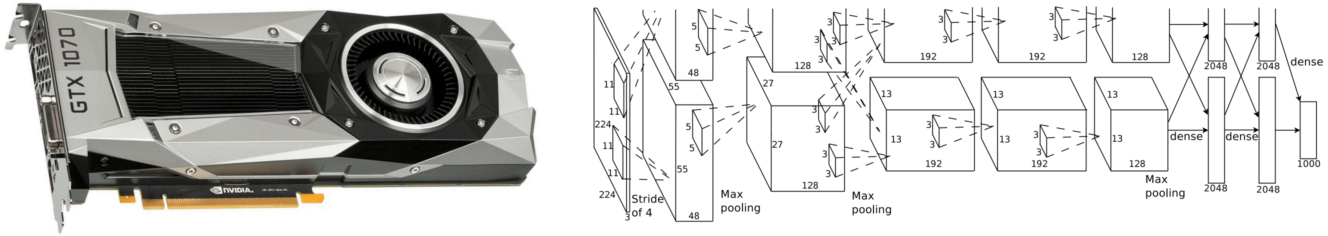
Backward: Compute gradient

Batch of
N images

Exchange gradients,
sum, update

Forward: compute loss

N / 2
images

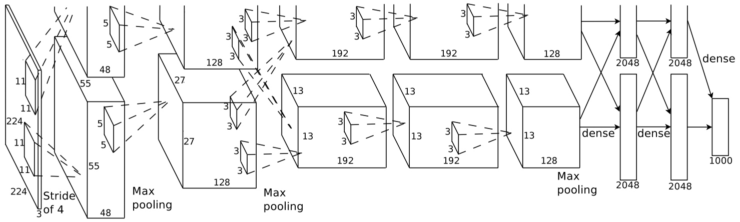


Backward: Compute gradient

GPUs only
communicate once per
iteration, and only
exchange grad params

Data Parallelism: Copy Model on each GPU, split data

N / K images



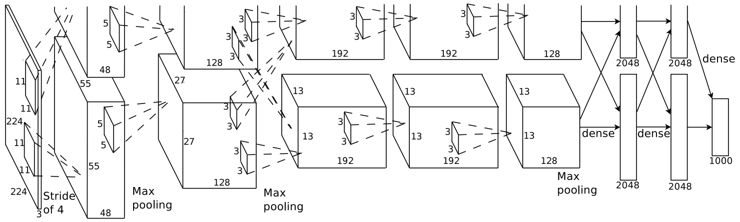
Batch of N images

Scale up to K GPUs (within and across servers)

…

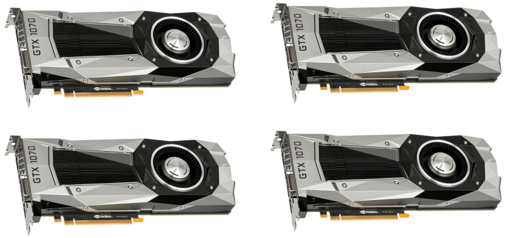
Main mechanism for distributing across many GPUs today

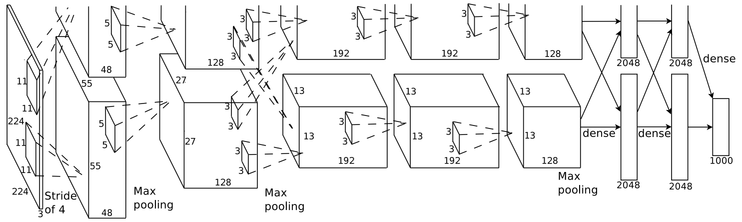
N / K images



Mixed Model + Data Parallelism

N / K images





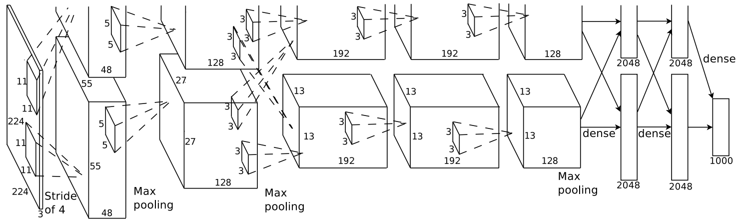
Batch of N images

Model parallelism **within** each server

...

Data parallelism **across** K servers

N / K images

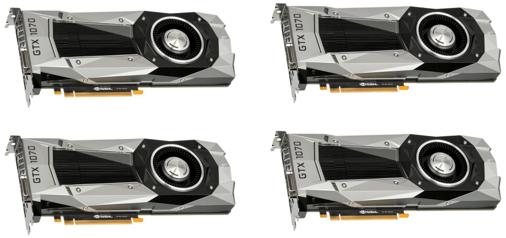


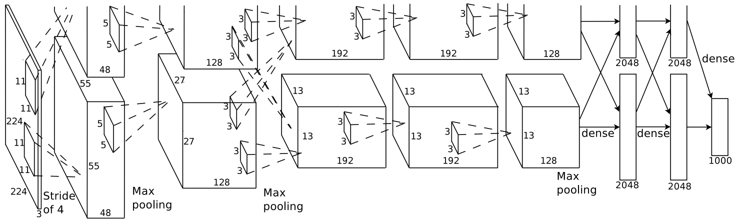
Example: https://devblogs.nvidia.com/training-bert-with-gpus/

Mixed Model + Data Parallelism

Problem: Need to train with very large minibatches!

N / K images





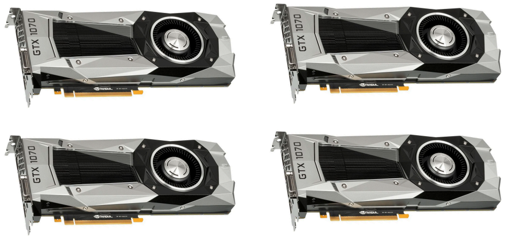
Batch of N images

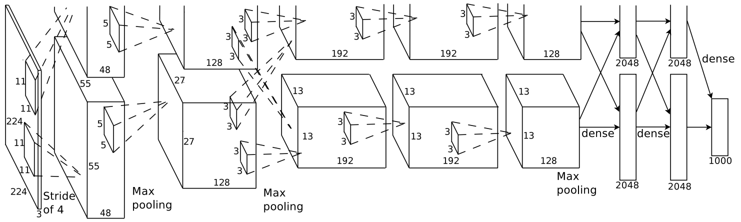
Model parallelism **within** each server

...

Data parallelism **across** K servers

N / K images



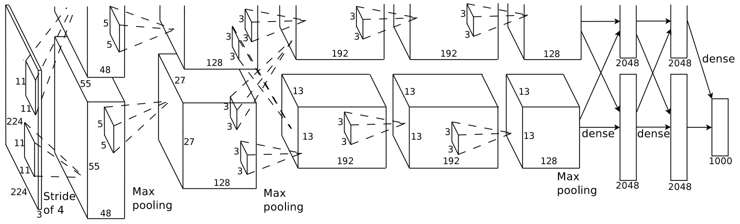


Example: https://devblogs.nvidia.com/training-bert-with-gpus/

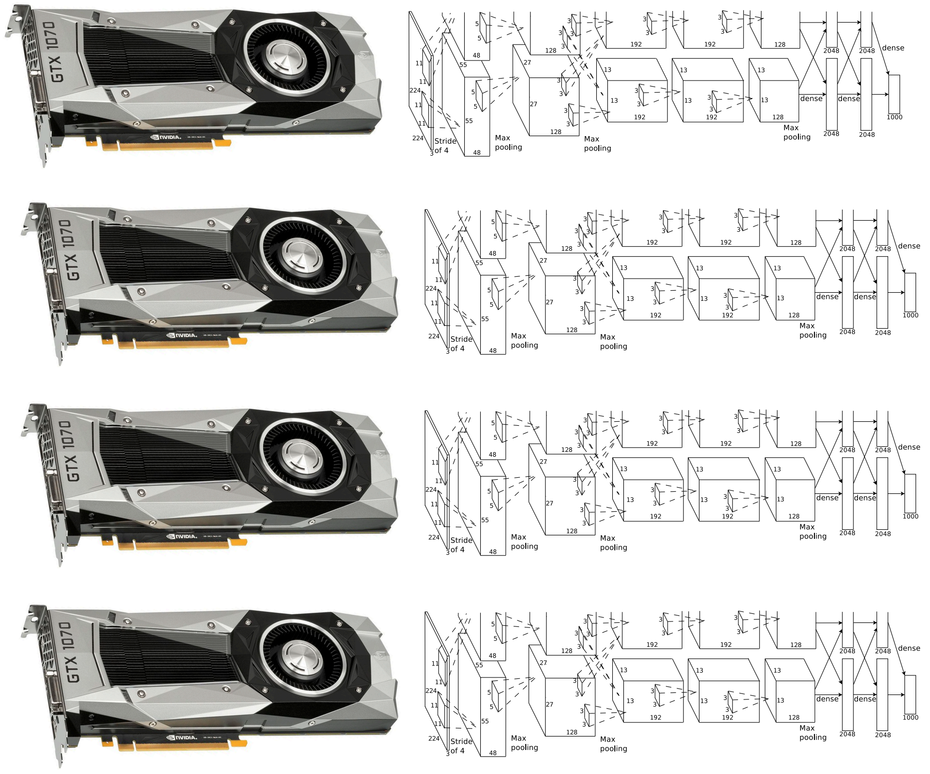
Large-Batch Training

Large-Batch Training

Suppose we can train a good model with one GPU



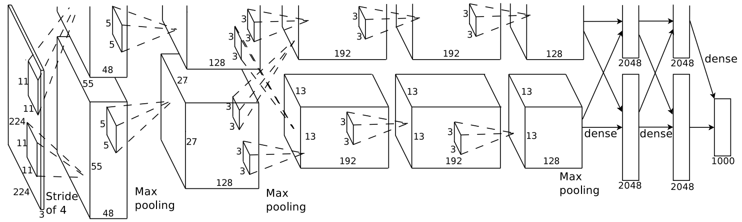
How to scale up to data-parallel training on K GPUs?



...

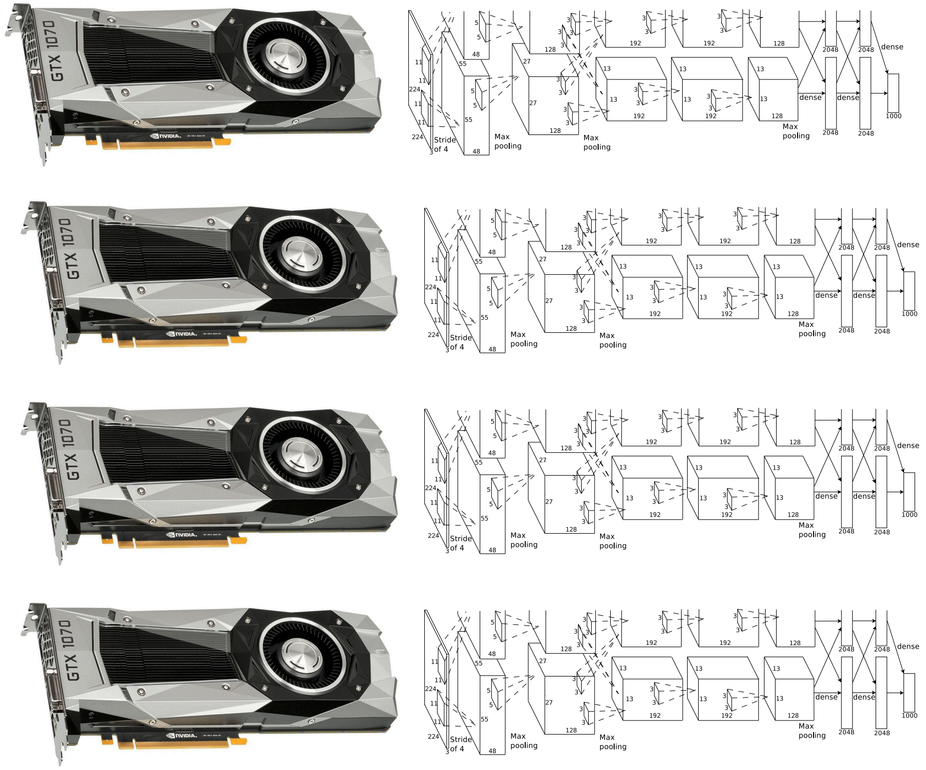
Large-Batch Training

Suppose we can train a good model with one GPU



Goal: Train for same number of epochs, but use larger minibatches. We want model to train K times faster!

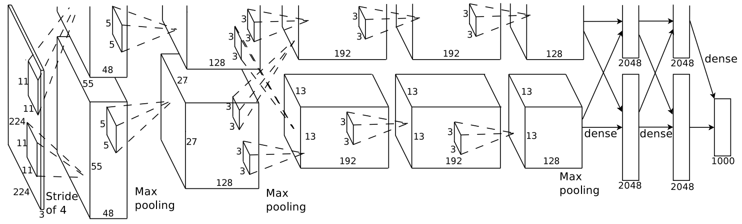
How to scale up to data-parallel training on K GPUs?



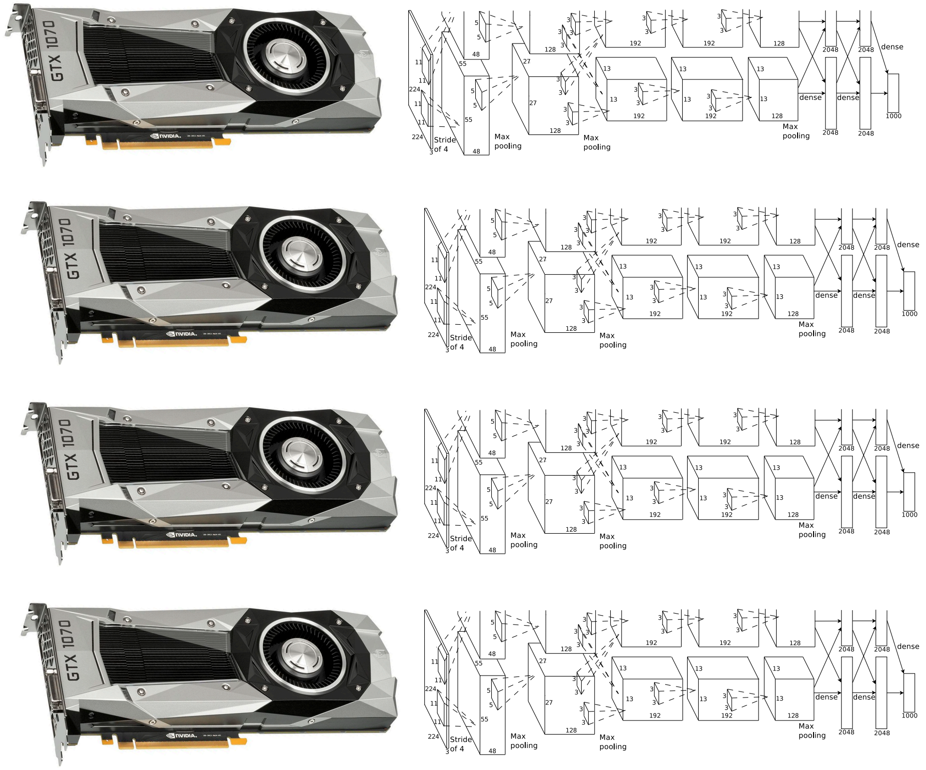
...

Large-Batch Training: Scale Learning Rates

Single-GPU model:
batch size N, learning rate α

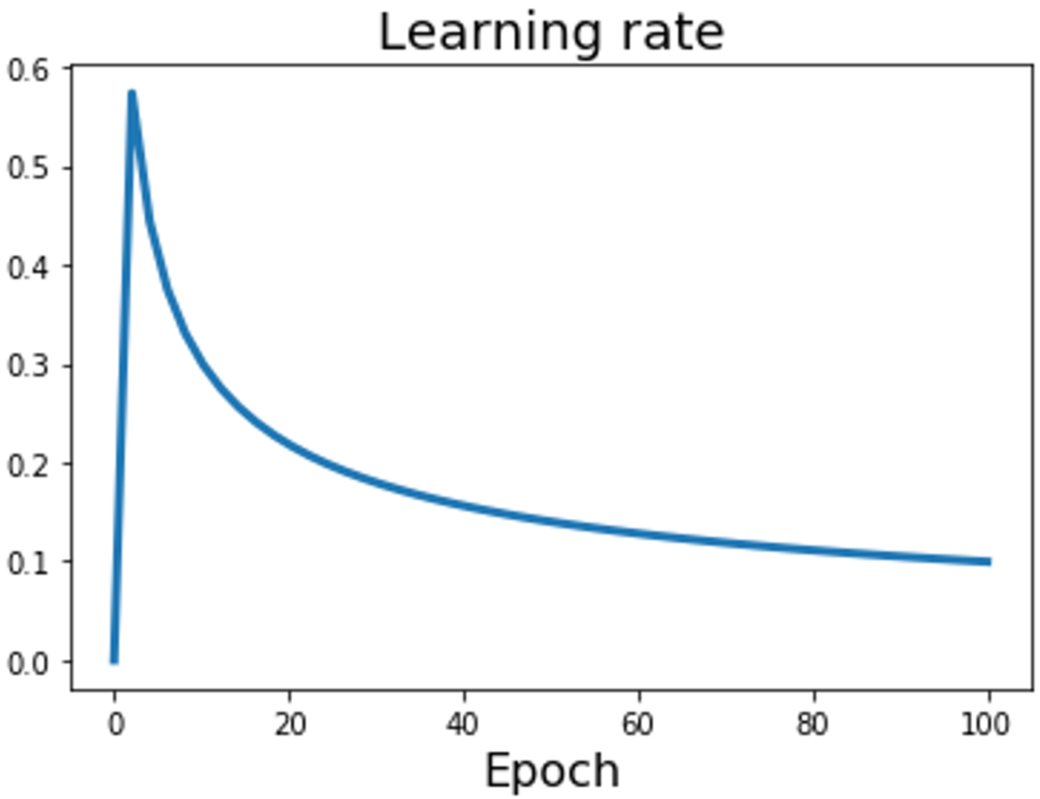


K-GPU model:
batch size KN, learning rate $K\alpha$



Alex Krizhevsky, “One weird trick for parallelizing convolutional neural networks”, arXiv 2014
Goyal et al, “Accurate, Large Minibatch SGD: Training ImageNet in 1 Hour”, arXiv 2017

Large-Batch Training: Learning Rate Warmup



High initial learning rates can make loss explode; linearly **increasing** learning rate from 0 over the first ~5000 iterations can prevent this

Goyal et al, "Accurate, Large Minibatch SGD: Training ImageNet in 1 Hour", arXiv 2017

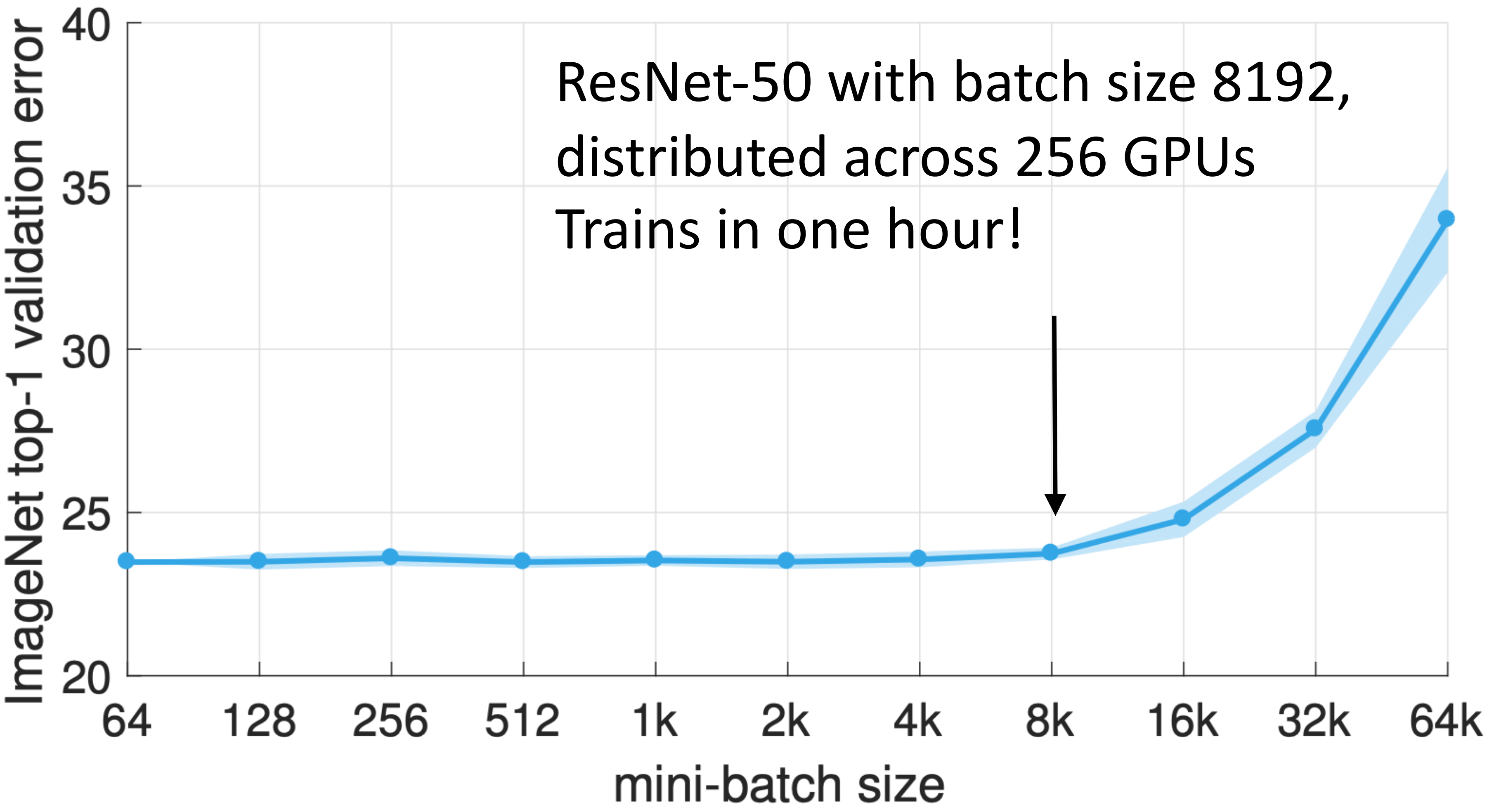
Large-Batch Training: Other Concerns

Be careful with **weight decay** and **momentum**, and **data shuffling**

For Batch Normalization, only normalize **within a GPU**

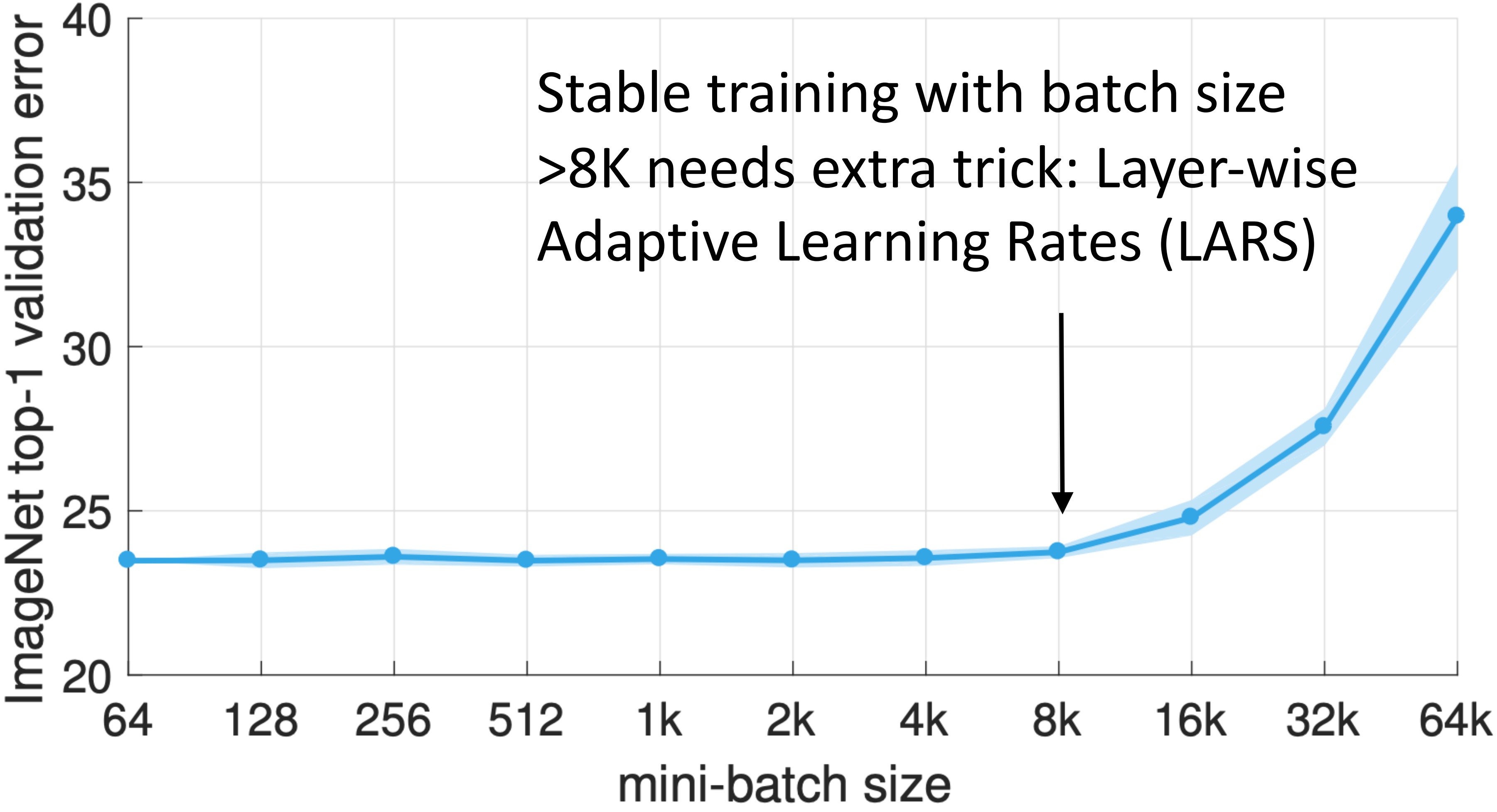
Goyal et al, "Accurate, Large Minibatch SGD: Training ImageNet in 1 Hour", arXiv 2017

Large-Batch Training: ImageNet in One Hour!



Goyal et al, "Accurate, Large Minibatch SGD: Training ImageNet in 1 Hour", arXiv 2017

Large-Batch Training: ImageNet in One Hour!



Goyal et al, “Accurate, Large Minibatch SGD: Training ImageNet in 1 Hour”, arXiv 2017

You et al, “Large Batch Training of Convolutional Networks”, arXiv 2017

Large-Batch Training

Goyal et al, "Accurate, Large Minibatch SGD: Training ImageNet in 1 Hour", 2017
Batch size: 8192; 256 P100 GPUs; 1 hour

Codreanu et al, "Achieving deep learning training in less than 40 minutes on imagenet-1k", 2017
Batch size: 12288; 768 Knight's Landing devices; 39 minutes

You et al, "ImageNet training in minutes", 2017
Batch size: 16000; 1600 Xeon CPUs; 31 minutes

Akiba et al, "Extremely Large Minibatch SGD: Training ResNet-50 on ImageNet in 15 Minutes", 2017
Batch size: 32768; 1024 P100 GPUs; 15 minutes

MLPerf v0.7 (NVIDIA): 1840 A100 GPUs; **46 seconds**

MLPerf v0.7 (Google): TPU-v3-8192; Batch size 65536; **27 seconds!**

MLPerf
https://mlperf.org/

Recap

1. **One time setup**
   Activation functions, data preprocessing, weight initialization, regularization
2. **Training dynamics**
   Learning rate schedules;
   hyperparameter optimization
3. **After training**
   Model ensembles, transfer learning,
   large-batch training

Last Time

Today

Next Time:
Recurrent Neural Networks