

### This Week in Al



Image from nvidia

### **Topics**

#### Optimization revisited

- ► Gradient descent improvements
- ► Learning rate scheduling

#### Normalization layers

► Batch & layer normalization

### Optimization vs. machine learning

- ► Underfitting & overfitting
- ► Data augmentation



We already know how to train CNNs (for classification)

- ightharpoonup Calculate (cross-entropy) loss  $L(\theta)$  on training data
- lacktriangle Compute  $abla L(oldsymbol{ heta})$  using backpropagation
- ightharpoonup Use gradient descent to update heta

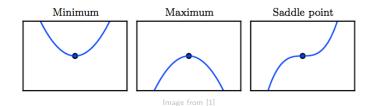
Need some tweaks to make this pipeline practicable



Gradient Descent

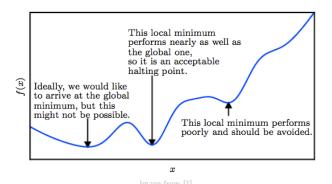
Gradient descent update rule is  $\theta = \theta - \alpha \nabla L(\theta)$ 

- ▶ Algorithm stops if  $\nabla L(\theta) = \mathbf{0}$  (at critical points)
- ▶ But should only stop at global minimum ...



#### Gradient Descent

#### ... or a "good" local minimum



Luckily studies show that in deep learning

- ► There are few (if any) local minima
- ► Local minima are "good" in above sense

Simple gradient descent thus works in theory but is

- ► Too expensive to compute with large datasets
- Too slow around critical points



Recall that  $L(\theta)$  is average over S training samples

- ightharpoonup Time complexity per iteration increases linearly with S
- ▶ Problem with large datasets (need many iterations)

To solve this problem we process the training set

- ightharpoonup In minibatches of size S (one per iteration)
- Using minibatch loss and gradient as estimators

One full run through training set is called an epoch

► Training usually takes many epochs



Time complexity for single iteration independent of dataset size

Resulting algorithm called minibatch gradient descent

► Or stochastic gradient descent (SGD)

 ${\cal S}$  varies between 1 and a few hundred samples

- ▶ Usually  $S = 2^n$ , e.g. 32, 64, 128, 256
- ▶ Powers of 2 for efficiency



#### Decreasing S also decreases

- Computation time per iteration
- ► Memory required on GPU (minibatch processed as whole)
- Accuracy of gradient estimate

#### Minibatch gradients are noisy estimates

- Gives gradient descent ability to escape critical points
- Can improve generalization
- ► Makes gradient descent non-deterministic



Important to sample minibatches randomly

► To break (possible) ordering in training set

Standard approach in practice

- Shuffle training set before every epoch
- Process sequentially in minibatches

Always use minibatch gradient descent



#### Gradient descent ignores information from previous iterations

► Slows down convergence

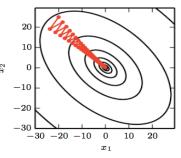


Image from [1]

Use exponential moving average of gradients for direction  ${\bf v}$ 

► Influence of older gradients decays exponentially

Improves speed of convergence by

- Dampening oscillations (previous slide)
- Increasing step size dynamically



Iteration of gradient descent with momentum

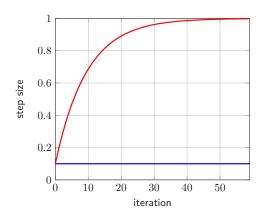
- Update velocity  $\mathbf{v} = \beta \mathbf{v} \alpha \nabla L(\boldsymbol{\theta})$
- ▶ Update parameters  $\theta = \theta + \mathbf{v}$

Hyperparameter  $\beta \in [0,1)$  called momentum

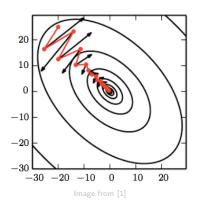
▶ Defines decay speed and maximum step size



Maximum speedup at constant gradient is  $1/(1-\beta)$ 



#### Momentum dampens oscillations



Nesterov Momentum

Evaluate gradient at  $heta+{f v}$  instead of heta

Iteration of gradient descent with Nesterov momentum

- ▶ Update velocity  $\mathbf{v} = \beta \mathbf{v} \alpha \nabla L(\boldsymbol{\theta} + \mathbf{v})$
- ▶ Update parameters  $\theta = \theta + \mathbf{v}$

Performance often slightly better than momentum

- Usually good idea to use this variant
- ▶ Setting  $\beta = 0.9$  is usually fine

## Optimization Revisited Remaining Limitations

Gradient descent step size depends on gradient magnitude

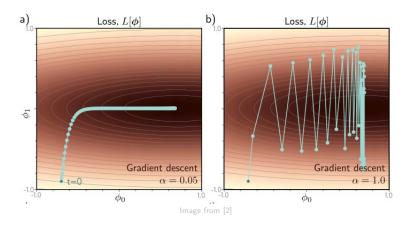
- ► Small gradients, small parameter adjustments
- Problem if gradient magnitudes vary significantly

Makes it impossible to chose  $\alpha$  such that

- ▶ We make progress in all directions
- Optimization remains stable



### Optimization Revisited Remaining Limitations



# Optimization Revisited RMSProp

#### RMSProp aims to address this limitation

- ► Adapt learning rate for each parameter
- Based on its variance

### Update step (initially $\mathbf{n}=\mathbf{0}$ )

$$\mathbf{n} = \beta_2 \mathbf{n} + (1 - \beta_2) \nabla^2 L(\boldsymbol{\theta})$$

#### Adam combines momentum and RMSProp

Update step (initially  $\mathbf{m}=\mathbf{n}=\mathbf{0})$ 

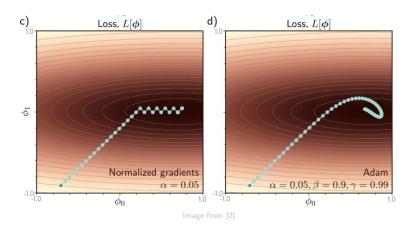
$$\mathbf{m} = \beta_1 \mathbf{m} + (1 - \beta_1) \nabla L(\boldsymbol{\theta})$$

$$\mathbf{n} = \beta_2 \mathbf{n} + (1 - \beta_2) \nabla^2 L(\boldsymbol{\theta})$$

$$\mathbf{m} = \mathbf{m}/(1 - \beta_1^t)$$

$$\mathbf{n} = \mathbf{n}/(1 - \beta_2^t)$$

$$\theta = \theta - \alpha \mathbf{m} / (\sqrt{\mathbf{n}} + \epsilon)$$



#### Adam works well in many scenarios

- ► Use as default optimizer
- ▶ Defaults for  $\beta_1$  and  $\beta_2$  are usually fine
- ▶ Tune  $\alpha$  if feasible, or if not ...  $\odot$



3e-4 is the best learning rate for Adam, hands down.

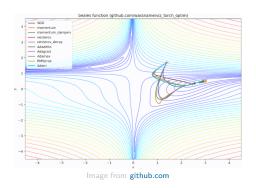
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**Alternatives** 

#### Path finding comparison on challenging f

▶ Different learning rates, so speed not comparable



Learning rate  $\alpha$  is important with any optimizer

▶ Influences training time & quality of optimization

Studies show  $\alpha$  should be varied during training

► To achieve both high speed and quality

Different strategies (schedulers) exist

▶ PyTorch: torch.optim.lr\_scheduler module

### A simple strategy is to

- ightharpoonup Start with some base learning rate  $\alpha$
- ▶ Set  $\alpha = \alpha/n$  if loss no longer decreases significantly
- torch.optim.lr\_scheduler.ReduceLROnPlateau
- ightharpoonup Common values for n are 2, 5, 10

#### Idea is to

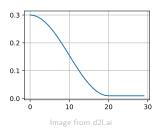
- Make fast progress initially (large  $\alpha$ )
- ightharpoonup Be more careful later (smaller  $\alpha$ )



Most schedulers adapt  $\alpha$  based on current epoch count

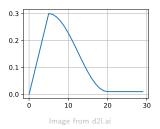
A popular variant is cosine decay

- lacktriangle Ensures lpha does not decrease too fast initially
- torch.optim.lr\_scheduler.CosineAnnealingLR



#### Warmup can be helpful in combination (e.g. Transformers)

- $\triangleright$  Start with small  $\alpha$
- ► Increase (e.g. linearly) for a few epochs
- ► Then decrease again (e.g. via cosine scheduling)



#### Cyclic variants also exist

► Repeat above pattern multiple times

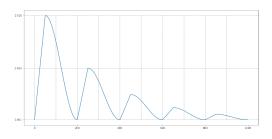


Image from github.com/katsura-jp

Always use learning rate scheduling

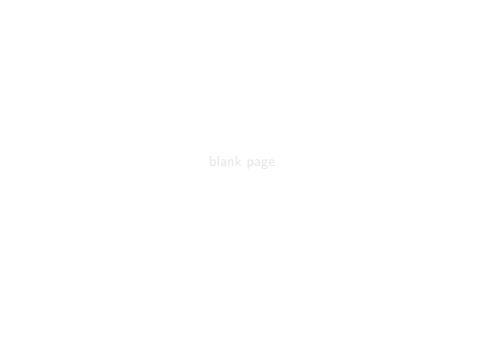
The ReduceLROnPlateau strategy is a solid default

- ► More intuitive than other variants
- ▶ No knowledge of sensible total epoch count needed

Other strategies may or may not work better

Depends on network architecture, optimizer, data, etc.

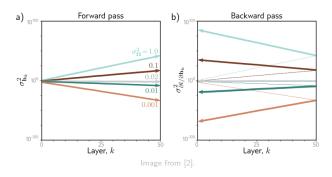




## Normalization Layers Motivation

#### Recall that deep networks are prone to vanishing/exploding signals

► Chained multiplications



### Normalization Layers

#### To avoid this we

- Initialize parameters carefully (previous lecture)
- ► Normalize input images

#### Standard image normalization method

- ► Subtract per-channel mean of training set
- Divide by per-channel standard deviation

#### This ensures a stable signal only initially though

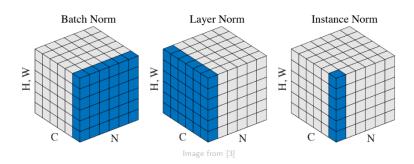
► Weights change during training



### Normalization Layers Motivation

We want normalization built into our networks

- ► By adding normalization layers
- ▶ Batch normalization is most popular method for CNNs



### Batch normalization [4] normalizes minibatch statistics

Input: Values of x over a mini-batch:  $\mathcal{B} = \{x_{1...m}\}$ ; Parameters to be learned:  $\gamma$ ,  $\beta$ Output:  $\{y_i = \mathrm{BN}_{\gamma,\beta}(x_i)\}$   $\mu_{\mathcal{B}} \leftarrow \frac{1}{m} \sum_{i=1}^m x_i \qquad \text{// mini-batch mean}$   $\sigma_{\mathcal{B}}^2 \leftarrow \frac{1}{m} \sum_{i=1}^m (x_i - \mu_{\mathcal{B}})^2 \qquad \text{// mini-batch variance}$   $\hat{x}_i \leftarrow \frac{x_i - \mu_{\mathcal{B}}}{\sqrt{\sigma_{\mathcal{B}}^2 + \epsilon}} \qquad \text{// normalize}$   $y_i \leftarrow \gamma \hat{x}_i + \beta \equiv \mathrm{BN}_{\gamma,\beta}(x_i) \qquad \text{// scale and shift}$ 

### Normalization Layers

**Batch Normalization** 

#### Steps (variant for conv layers)

- lacktriangle Estimate per-channel means  $\mu_c$  and variances  $\sigma_c^2$
- Using current minibatch to approximate training set
- Normalize each channel as in previous slide
- Multiply channels by  $\gamma_c$ , add  $\beta_c$

Last step ensures normalization can be skipped if sensible

▶ Identity function if  $\gamma_c = \sigma_c$  and  $\beta_c = \mu_c$ 

### Normalization Layers

**Batch Normalization** 

#### Advantages

- ► Well-behaved signals (enables deeper networks)
- ► Smoother loss functions (allows higher learning rates)
- ► Has regularizing effect due to noisy minibatch statistics

#### Add after every conv and linear hidden layer

- ► Usually before the activation function
- PyTorch: torch.nn.BatchNorm2d (conv version)
- Shuffle training set before every epoch (regularization)



### Normalization Layers

**Batch Normalization** 

#### What about after training?

- ► Inference usually done on single samples
- ▶ Not possible to compute minibatch statistics

#### Thus these statistics are

- Aggregated during training (moving averages)
- Used after training for normalization



# Normalization Layers Layer Normalization

#### Layer normalization [6] is also popular

- ▶ Normalization done per-sample instead of per-channel
- ► Works with single samples (no moving averages needed)
- Used in Transformers (later) and some modern CNNs

#### Stick with batch normalization for CNNs though

Layer normalization often performs worse



## Normalization Layers Differences (2D Case)

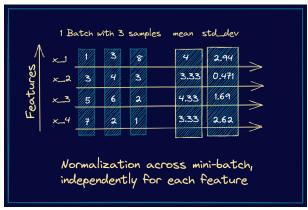


Image from pinecone.io



### Normalization Layers

Differences (2D Case)

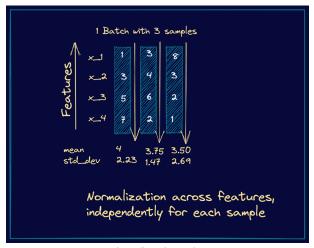
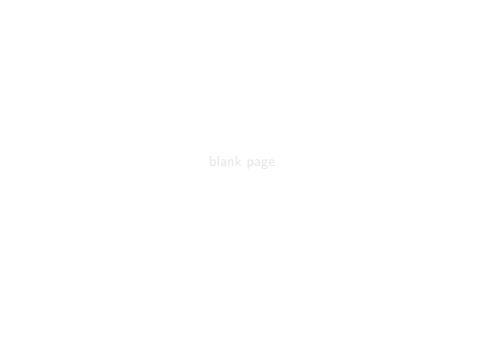


Image from pinecone.io





We covered training from an optimization perspective

- ► Find parameters that minimize training loss
- ► Known as empirical risk minimization

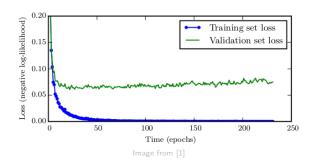
#### Prone to overfitting

- Training data must capture underlying distribution well
- Usually not the case in image analysis



#### Typical example of overfitting

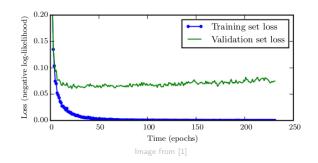
- Training loss decreases steadily
- ► Validation loss remains high (gets worse)





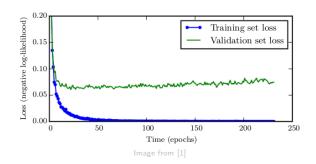
So optimization was successful (loss  $\approx 0$ )

- But disappointing validation/test performance
- Due to ability to generalize well to unseen data



In machine learning our actual goals are

- ► Low training loss (avoid underfitting)
- ► Small gap to validation loss (avoid overfitting)



#### To (hopefully) achieve this we

- ► Minimize the training loss (we have to)
- ▶ While monitoring training & validation performance
- And combat overfitting

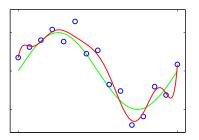
#### Monitoring losses can be unintuitive

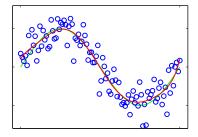
- ► Can be hard to interpret (e.g. cross-entropy loss)
- Training loss can be affected by regularization (next lecture)
- Use suitable performance measures instead (e.g. accuracy)



Best way to improve generalization: more training data

▶ But in practice data are limited





Create meaningful fake training data (training data augmentation)

- ► Apply transformations to training samples
- ► That have no effect on output (e.g. class label)







mage adapted from youtube

Can be done online, no need to store transformed samples

► Apply transformations during minibatch generation

#### Common transformations

- ► Random cropping
- ightharpoonup Horizontal mirroring with probability 0.5
- Random similarity or affine transforms
- Random contrast, brightness, sharpness changes

PyTorch: torchvision.transforms



#### Mixup is a powerful extension

► Randomly mix two training images and their labels

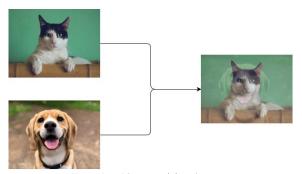


Image adapted from towardsdatascience.com



# Optimization vs. Machine Learning Regularization

To avoid overfitting we have two options

- ▶ Use a network with just enough capacity not to overfit
- Prevent a network with more capacity from overfitting

Option 2 is always preferred in practice

- Leads to better performance
- ▶ We will see how to implement this in next lecture



## Bibliography

- [1] Goodfellow et al. Deep Learning. 2016
- [2] Prince. Understanding Deep Learning. 2023
- [3] Wu & He. Group Normalization. 2022
- [4] loffe & Szegedy. Batch Normalization. 2015
- [5] Srivastava et al. Dropout. 2014
- [6] Lei Ba et al. Layer Normalization. 2016

