

#### **Topics**

#### Optimization

- Gradient descent
- Momentum

For training any parametric model, we need

- A loss function
- ► An optimization algorithm

We'll use cross-entropy loss (previous lecture)

#### Recall that cross-entropy loss $L(\theta)$

- Measures performance of classifier  $\mathbf{w} = f(\mathbf{x}; \boldsymbol{\theta})$
- $lackbox{ On some dataset } \mathcal{D} = \{(\mathbf{x}_s, \mathbf{w}_s)\}_{s=1}^S$
- lacktriangle With respect to parameters  $oldsymbol{ heta}$

 $L(\boldsymbol{\theta})$  measures how dissimilar softmax( $\mathbf{w}$ ) and  $\mathbf{w}_s$  are

ightharpoonup softmax( $\mathbf{w}$ ) and  $\mathbf{w}_s$  are discrete probability distributions

We want to minimize loss (dissimilarity) by changing heta

► For this we need an optimization algorithm

#### $L({m heta})$ is not linear in ${m heta}$

► Need a nonlinear optimization algorithm

We'll use gradient descent (steepest descent)

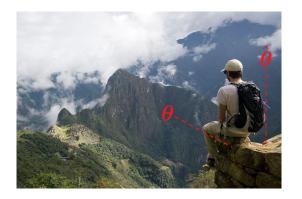
▶ Most popular algorithm in Deep Learning

Assume terrain corresponds to  $L(\theta)$  with  $\dim(\theta) = 2$ 



# Optimization Problem Definition

How do I get from location  $\theta$  to location of minimum  $\hat{\theta}$ ?



#### Without actually seeing $L(\theta)$ ?



# Optimization Gradient Descent

Feel slope with feet, step in direction that feels steepest



# Optimization Gradient Descent

Again and again, until I cannot get lower





#### Iterative algorithm

In every iteration we

- ▶ Compute gradient  $\theta' = \nabla L(\theta)$
- ▶ Update parameters  $\theta = \theta \alpha \theta'$

Hyperparameter  $\alpha>0$  is called learning rate

▶ Final step size is  $\alpha \| \boldsymbol{\theta}' \|$ 



Let  $f(x_1, \ldots, x_n)$  be a differentiable, real-valued function

The partial derivative  $f_{x_i}$  of f with respect to  $x_i$ 

▶ Is also a real-valued function  $f_{x_i}(x_1, \dots, x_n)$ 

 $f_{x_i}(\mathbf{x})$  encodes

- ▶ How fast f changes with argument  $x_i$
- At some location x



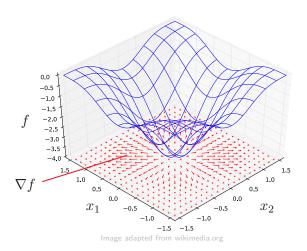
#### Gradient $\nabla f$ is vector of all partial derivatives of f

- $\triangleright \nabla f = (f_{x_1}, \dots, f_{x_n})$
- ▶ Vector-valued function  $\mathbb{R}^n \mapsto \mathbb{R}^n$

$$\nabla f(\mathbf{x}) = (f_{x_1}(\mathbf{x}), \dots, f_{x_n}(\mathbf{x}))$$
 encodes

- ▶ How fast f changes with all arguments  $x_1 \cdots x_n$
- At some location x





 $\nabla f(\mathbf{x})$  specifies how f changes locally at  $\mathbf{x}$ 

- ▶ Points in direction of greatest increase
- ► Norm equals magnitude of increase

Exactly what we need to minimize  $\boldsymbol{L}$ 

- lacktriangle Compute direction of greatest increase  $abla L(m{ heta})$
- Move in the opposite direction



We stop if  $\nabla L(\boldsymbol{\theta}) = \mathbf{0}$  (if norm is 0)

- ▶ No information where to go next
- ▶ L is flat at current location
- ▶ The case if we are at  $\hat{\theta}$  (but not only then)

#### Simple and general algorithm

ightharpoonup Requires only that f is differentiable, real-valued

#### Several (possible) limitations

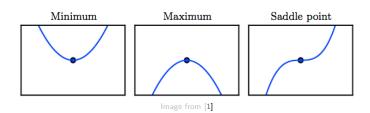
- ightharpoonup Performs poorly for many f
- But generally well for loss functions of neural networks



### Gradient Descent Limitations – Critical Points

Algorithm stops if  $\nabla L(\boldsymbol{\theta}) = \mathbf{0}$ 

- ► Applies to all critical points, not only minimum
- ► Should stop only at minimum



### Gradient Descent Limitations - Critical Points

Could look at second derivatives of L (Hessian)

- Describes curvature of L
- ► Second-order optimization methods do this

For loss functions of large neural networks

- Estimating Hessian very expensive
- Critical points usually not problematic



## Gradient Descent Limitations – Local Minima

Algorithm stops at first minimum as  $\nabla L(\boldsymbol{\theta}) = \mathbf{0}$ 

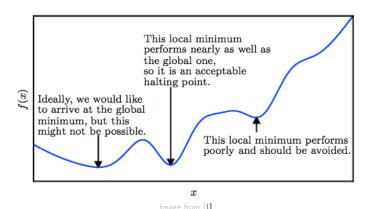
- $\blacktriangleright$  But L generally has several local minima
- Algorithm usually finds only a local minimum

For loss functions of large neural networks

- ► Most local minima are close to global minimum
- So local minima usually not problematic

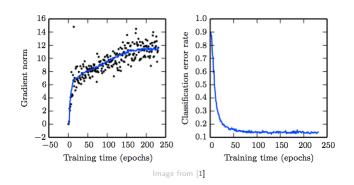


### Gradient Descent Limitations – Local Minima



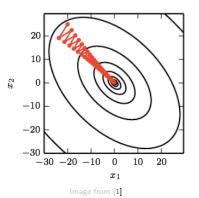
## Gradient Descent Limitations – Local Minima

In practice we don't even arrive at any critical point



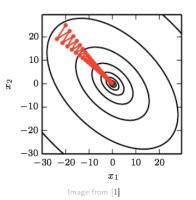
### Gradient Descent Limitations – Poorly Conditioned Hessian

Very different curvature in different directions (canyon-like)



### Gradient Descent Limitations – Poorly Conditioned Hessian

Gradient descent wastes time jumping between canyon walls



#### Momentum improves speed of convergence by

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

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

Influence of older gradients decays exponentially



Iteration of gradient descent with momentum

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

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

► Defines decay speed and maximum step size

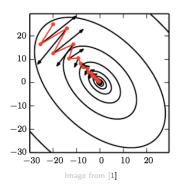
 ${f v}$  builds up momentum if successive gradients are similar

► Improves speed of convergence

Maximum step size is  $\alpha \|\mathbf{g}\|/(1-\beta)$ 

- ► Assuming the gradient is always g
- At  $\beta = 0.9$  maximum increase by factor of 10

Red is path, black are steepest descent directions



Evaluate gradient at  $oldsymbol{ heta}+\mathbf{v}$  instead of  $oldsymbol{ heta}$ 

Iteration of gradient descent with Nesterov momentum

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

Often works better than standard momentum



Before we can apply gradient descent, we must know

- ▶ How to select  $\mathcal{D}$  (data for loss function)
- ightharpoonup How to initialize parameters heta properly
- ▶ How to actually compute gradient

We'll cover this in next lecture



#### Bibliography

[1] Deep learning, 2016, [Online]. Available: http://www.deeplearningbook.org.

