CMSC 491/691

Lecture 9

Neural Network Optimization



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Neural Network Optimization



Some slides from Owens, Jayasuriya, Karpathy



CMSC 491/691



Stacking layers



h = "hidden units"



I know a guy who knows a guy

Computation in a neural net – Full Layer



How do we learn the parameters?



Computation has a simple form

- Composition of linear functions with nonlinearities in between
- E.g. matrix multiplications with ReLU, $max(0, \mathbf{x})$ afterwards
- Do a matrix multiplication, set all negative values to 0, repeat

But where do we get the weights from?

Training neural networks

Let's start easy

world's smallest neural network! (a "perceptron")



$$y = wx$$

(a.k.a. line equation, linear regression)

Training a Neural Network

Given a set of samples and a Perceptron $\{x_i, y_i\}$ $y = f_{ ext{PER}}(x; w)$

Estimate the parameter of the Perceptron

w

Given training data:



What do you think the weight parameter is?

$$y = wx$$

Given training data:



What do you think the weight parameter is?

$$y = wx$$

not so obvious as the network gets more complicated so we use ...

An Incremental Learning Strategy

(gradient descent)

Given several examples

$$\{(x_1, y_1), (x_2, y_2), \dots, (x_N, y_N)\}$$

and a perceptron $\hat{y} = wx$

An Incremental Learning Strategy

(gradient descent)

Given several examples

$$\{(x_1, y_1), (x_2, y_2), \dots, (x_N, y_N)\}$$

and a perceptron $\hat{y} = wx$

Modify weight $\,w$ such that $\,\hat{y}\,$ gets 'closer' to $\,y\,$

An Incremental Learning Strategy

(gradient descent)

Given several examples

$$\{(x_1, y_1), (x_2, y_2), \dots, (x_N, y_N)\}$$

and a perceptron $\hat{y} = wx$





SHEN COMIX



Zero-One Loss $\ell(\hat{y}, y) = \mathbf{1}[\hat{y} = y]$

Hinge Loss $\ell(\hat{y}, y) = \max(0, 1 - y \cdot \hat{y})$



Backpropagation

Geoff Hinton after writing the paper on backprop in 1986



Backpropagation



 $\frac{d\mathcal{L}}{dw}$... is the rate at which **this** will change...

$$\mathcal{L} = \frac{1}{2}(y - \hat{y})^2 \checkmark$$

the loss function

... per unit change of this



Let's compute the derivative...

Compute the derivative

$$egin{aligned} &rac{d\mathcal{L}}{dw} = rac{d}{dw}iggl\{rac{1}{2}(y-\hat{y})^2iggr\}\ &= -(y-\hat{y})rac{dwx}{dw}\ &= -(y-\hat{y})x =
abla w \end{aligned}$$

That means the weight update for **gradient descent** is:

$$w = w -
abla w$$
 move in direction of negative gradient $= w + (y - \hat{y})x$

Gradient Descent (world's smallest perceptron) For each sample $\{x_i, y_i\}$ 1. Predict a. Forward pass $\hat{y} = wx_i$ $\mathcal{L}_i = rac{1}{2}(y_i - \hat{y})^2$ b.Compute Loss 2. Update $\frac{d\mathcal{L}_i}{dw} = -(y_i - \hat{y})x_i = \nabla w$ a. Back Propagation $w = w - \nabla w$ b. Gradient update

multi-layer perceptron



function of FOUR parameters and FOUR layers!







 $a_1 = w_1 \cdot x + b_1$



 $a_1 = w_1 \cdot x + b_1$



$$a_1 = w_1 \cdot x + b_1$$
$$a_2 = w_2 \cdot f_1(w_1 \cdot x + b_1)$$



$$a_1 = w_1 \cdot x + b_1$$

 $a_2 = w_2 \cdot f_1(w_1 \cdot x + b_1)$



$$a_1 = w_1 \cdot x + b_1$$

 $a_2 = w_2 \cdot f_1(w_1 \cdot x + b_1)$
 $a_3 = w_3 \cdot f_2(w_2 \cdot f_1(w_1 \cdot x + b_1))$



$$a_1 = w_1 \cdot x + b_1$$

 $a_2 = w_2 \cdot f_1(w_1 \cdot x + b_1)$
 $a_3 = w_3 \cdot f_2(w_2 \cdot f_1(w_1 \cdot x + b_1))$



$$egin{aligned} a_1 &= w_1 \cdot x + b_1 \ a_2 &= w_2 \cdot f_1(w_1 \cdot x + b_1) \ a_3 &= w_3 \cdot f_2(w_2 \cdot f_1(w_1 \cdot x + b_1)) \ y &= f_3(w_3 \cdot f_2(w_2 \cdot f_1(w_1 \cdot x + b_1))) \end{aligned}$$
Entire network can be written out as one long equation

$$y = f_3(w_3 \cdot f_2(w_2 \cdot f_1(w_1 \cdot x + b_1)))$$

We need to train the network: What is known? What is unknown? Entire network can be written out as a long equation

$$y = f_3(w_3 \cdot f_2(w_2 \cdot f_1(w_1 \cdot x + b_1)))$$

We need to train the network: What is known? What is unknown? Entire network can be written out as a long equation



What is known? What is unknown?

Learning an MLP

Given a set of samples and a MLP $\{x_i, y_i\}$ $y = f_{ ext{MLP}}(x; heta)$

Estimate the parameters of the MLP

$$heta = \{f, w, b\}$$

Gradient Descent

For each **random** sample $\{x_i, y_i\}$ 1. Predict

a. Forward pass $\hat{y} = f_{\mathrm{MLP}}(x_i; \theta)$

b.Compute Loss

2.Update

a.Back Propagation

b.Gradient update

$$\frac{\partial \mathcal{L}}{\partial \theta}$$
 vector of parameter partial derivatives
$$\theta \leftarrow \theta - \eta \nabla \theta$$

vector of parameter update equations

So we need to compute the partial derivatives

$$\frac{\partial \mathcal{L}}{\partial \boldsymbol{\theta}} = \left[\frac{\partial \mathcal{L}}{\partial w_3} \frac{\partial \mathcal{L}}{\partial w_2} \frac{\partial \mathcal{L}}{\partial w_1} \frac{\partial \mathcal{L}}{\partial b} \right]$$



According to the chain rule...

$$\frac{\partial L}{\partial w_3} = \frac{\partial L}{\partial f_3} \frac{\partial f_3}{\partial a_3} \frac{\partial a_3}{\partial w_3}$$











$$L(y, \hat{y})$$

$$\frac{\partial L}{\partial w_3} = \frac{\partial L}{\partial f_3} \frac{\partial f_3}{\partial a_3} \frac{\partial a_3}{\partial w_3}$$
$$= -\eta (y - \hat{y}) \frac{\partial f_3}{\partial a_3} \frac{\partial a_3}{\partial w_3}$$
Just the partial derivative of L2 loss



$$L(y, \hat{y})$$

$$\frac{\partial L}{\partial w_3} = \frac{\partial L}{\partial f_3} \frac{\partial f_3}{\partial a_3} \frac{\partial a_3}{\partial w_3}$$
$$= -\eta (y - \hat{y}) \frac{\partial f_3}{\partial a_3} \frac{\partial a_3}{\partial w_3}$$
Let's use a Sigmoid function

$$\frac{ds(x)}{dx} = s(x)(1 - s(x))$$

rest of the network
$$f_2 - w_3 \longrightarrow a_3 \mid f_3 \longrightarrow \hat{y} \qquad L(y, \hat{y})$$

$$L(y, \hat{y})$$

$$egin{aligned} rac{\partial L}{\partial w_3} &= rac{\partial L}{\partial f_3} rac{\partial f_3}{\partial a_3} rac{\partial a_3}{\partial w_3} \ &= -\eta (y-\hat{y}) rac{\partial f_3}{\partial a_3} rac{\partial a_3}{\partial w_3} \ &= -\eta (y-\hat{y}) f_3 (1-f_3) rac{\partial a_3}{\partial w_3} \ &= -\eta (y-\hat{y}) f_3 (1-f_3) rac{\partial a_3}{\partial w_3} \ &= -\eta (y-\hat{y}) f_3 (1-f_3) f_2 \end{aligned}$$



∂L _	∂L	∂f_3	∂a_3	∂f_2	∂a_2
$\overline{\partial w_2}$ –	$\overline{\partial f_3}$	$\overline{\partial a_3}$	$\overline{\partial f_2}$	$\overline{\partial a_2}$	$\overline{\partial w_2}$



$$\frac{\partial L}{\partial w_2} = \underbrace{\frac{\partial L}{\partial f_3} \frac{\partial f_3}{\partial a_3} \frac{\partial a_3}{\partial f_2} \frac{\partial f_2}{\partial a_2} \frac{\partial a_2}{\partial w_2}}_{\partial w_2}$$

already computed. re-use (<u>propagate</u>)! The chain rule says...



$$\frac{\partial L}{\partial w_1} = \frac{\partial L}{\partial f_3} \frac{\partial f_3}{\partial a_3} \frac{\partial a_3}{\partial f_2} \frac{\partial f_2}{\partial a_2} \frac{\partial a_2}{\partial f_1} \frac{\partial f_1}{\partial a_1} \frac{\partial a_1}{\partial w_1}$$

The chain rule says...



$$\frac{\partial L}{\partial w_1} = \left[\frac{\partial L}{\partial f_3} \frac{\partial f_3}{\partial a_3} \frac{\partial a_3}{\partial f_2} \frac{\partial f_2}{\partial a_2} \frac{\partial a_2}{\partial f_1} \frac{\partial f_1}{\partial a_1} \frac{\partial a_1}{\partial w_1} \right]_{\text{already computed.}}$$

re-use (propagate)!



$$\frac{\partial \mathcal{L}}{\partial w_3} = \frac{\partial \mathcal{L}}{\partial f_3} \frac{\partial f_3}{\partial a_3} \frac{\partial a_3}{\partial w_3} \\
\frac{\partial \mathcal{L}}{\partial w_2} = \frac{\partial \mathcal{L}}{\partial f_3} \frac{\partial f_3}{\partial a_3} \frac{\partial a_3}{\partial f_2} \frac{\partial f_2}{\partial a_2} \frac{\partial a_2}{\partial w_2} \\
\frac{\partial \mathcal{L}}{\partial w_1} = \frac{\partial \mathcal{L}}{\partial f_3} \frac{\partial f_3}{\partial a_3} \frac{\partial a_3}{\partial f_2} \frac{\partial f_2}{\partial a_2} \frac{\partial a_2}{\partial f_1} \frac{\partial f_1}{\partial a_1} \frac{\partial a_1}{\partial w_1} \\
\frac{\partial \mathcal{L}}{\partial b} = \frac{\partial \mathcal{L}}{\partial f_3} \frac{\partial f_3}{\partial a_3} \frac{\partial a_3}{\partial f_2} \frac{\partial f_2}{\partial a_2} \frac{\partial f_2}{\partial f_1} \frac{\partial a_1}{\partial a_1} \frac{\partial a_1}{\partial w_1}$$



$$\frac{\partial \mathcal{L}}{\partial w_3} = \frac{\partial \mathcal{L}}{\partial f_3} \frac{\partial f_3}{\partial a_3} \frac{\partial a_3}{\partial w_3}$$

$$\frac{\partial \mathcal{L}}{\partial w_2} = \frac{\partial \mathcal{L}}{\partial f_3} \frac{\partial f_3}{\partial a_3} \frac{\partial a_3}{\partial f_2} \frac{\partial f_2}{\partial a_2} \frac{\partial a_2}{\partial w_2}$$

$$\frac{\partial \mathcal{L}}{\partial w_1} = \frac{\partial \mathcal{L}}{\partial f_3} \frac{\partial f_3}{\partial a_3} \frac{\partial a_3}{\partial f_2} \frac{\partial f_2}{\partial a_2} \frac{\partial a_2}{\partial w_2}$$

$$\frac{\partial \mathcal{L}}{\partial f_3} = \frac{\partial \mathcal{L}}{\partial f_3} \frac{\partial f_3}{\partial a_3} \frac{\partial a_3}{\partial f_2} \frac{\partial f_2}{\partial a_2} \frac{\partial a_2}{\partial f_1} \frac{\partial f_1}{\partial a_1} \frac{\partial a_1}{\partial w_1}$$

$$\frac{\partial \mathcal{L}}{\partial b} = \frac{\partial \mathcal{L}}{\partial f_3} \frac{\partial f_3}{\partial a_3} \frac{\partial a_3}{\partial f_2} \frac{\partial f_2}{\partial a_2} \frac{\partial a_2}{\partial f_1} \frac{\partial f_1}{\partial a_1} \frac{\partial a_1}{\partial b}$$



$\partial \mathcal{L}$ _	$\partial \mathcal{L} \ \partial f_3 \ \partial a_3$	
$\overline{\partial w_3}$ –	$\overline{\partial f_3} \overline{\partial a_3} \overline{\partial w_3}$	
$\partial \mathcal{L}$ _	$\partial \mathcal{L} \partial f_3 \partial a_3 \partial f_2 \partial a_2$	
$\overline{\partial w_2}$ –	$\overline{\partial f_3}\overline{\partial a_3}\overline{\partial f_2}\overline{\partial a_2}\overline{\partial w_2}$	
$\partial \mathcal{L}$ _	$\partial \mathcal{L} \ \partial f_3 \ \partial a_3 \ \partial f_2 \ \partial a_2 \ \partial f_1 \ \partial f_1$	a_1
∂w_1	$\left[\overline{\partial f_3} \overline{\partial a_3} \overline{\partial f_2} \overline{\partial a_2} \overline{\partial f_1} \overline{\partial a_1} \overline{\partial a_2} \partial $	w_1
$\partial \mathcal{L}$	$\partial \mathcal{L} \; \partial f_3 \partial a_3 \partial f_2 \partial a_2 \partial f_1 \partial$	a_1
$\overline{\partial b}$ –	$\left[\overline{\partial f_3} \overline{\partial a_3} \overline{\partial f_2} \overline{\partial a_2} \overline{\partial f_1} \overline{\partial a_1} \overline{\partial a_2} \partial a_$	Эb

Gradient Descent

For each example sample $\{x_i, y_i\}$ 1. Predict $\hat{y} = f_{\text{MLP}}(x_i; \theta)$ a. Forward pass \mathcal{L}_i b. Compute Loss $rac{\partial \mathcal{L}}{\partial w_3} = rac{\partial \mathcal{L}}{\partial f_3} rac{\partial f_3}{\partial a_3} rac{\partial a_3}{\partial w_3}$ 2. Update $\frac{\partial \mathcal{L}}{\partial w_2} = \frac{\partial \mathcal{L}}{\partial f_3} \frac{\partial f_3}{\partial a_3} \frac{\partial a_3}{\partial f_2} \frac{\partial f_2}{\partial a_2} \frac{\partial a_2}{\partial w_2}$ a. Back Propagation $\frac{\partial \mathcal{L}}{\partial w_1} = \frac{\partial \mathcal{L}}{\partial f_3} \frac{\partial f_3}{\partial a_3} \frac{\partial a_3}{\partial f_2} \frac{\partial f_2}{\partial a_2} \frac{\partial a_2}{\partial f_1} \frac{\partial f_1}{\partial a_1} \frac{\partial a_1}{\partial w_1}$ $\frac{\partial \mathcal{L}}{\partial b} = \frac{\partial \mathcal{L}}{\partial f_3} \frac{\partial f_3}{\partial a_3} \frac{\partial a_3}{\partial f_2} \frac{\partial f_2}{\partial a_2} \frac{\partial a_2}{\partial f_1} \frac{\partial f_1}{\partial a_1} \frac{\partial a_1}{\partial b}$ $w_3 = w_3 - \eta \nabla w_3$ $w_2 = w_2 - \eta
abla w_2$ b. Gradient update $w_1 = w_1 - \eta \nabla w_1$

$$b = b - \eta
abla b$$

Gradient Descent

For each example sample $\{x_i, y_i\}$ 1. Predict a. Forward pass $\hat{y} = f_{\mathrm{MLP}}(x_i; \theta)$

- b.Compute Loss \mathcal{L}_i
- 2.Update
 - a.Back Propagation

 $rac{\partial \mathcal{L}}{\partial heta}$

vector of parameter partial derivatives

b.Gradient update

$$\theta \leftarrow \theta - \eta \frac{\partial \mathcal{L}}{\partial \theta}$$

vector of parameter update equations







negative gradient direction

$$\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} \ \textbf{-} \ \eta \frac{\partial \mathcal{L}}{\partial \boldsymbol{\theta}}$$

Step size: learning rate Too big: will miss the minimum Too small: slow convergence

Learning rate scheduling

- Use different learning rate at each iteration.
- Most common choice:

$$\eta_t = \frac{\eta_0}{\sqrt{t}}$$

Need to select initial learning rate η_0

More modern choice: Adaptive learning rates.

$$\eta_t = G\left(\left\{\frac{\partial L}{\partial \theta}\right\}_{i=0}^t\right)$$

Many choices for G (Adam, Adagrad, Adadelta).





Many other ways to perform optimization...

- Second order methods that use the Hessian (or its approximation): BFGS, **LBFGS**, etc.
- Currently, the lesson from the trenches is that well-tuned SGD+Momentum is very hard to beat for CNNs.
- No consensus on Adam etc.: Seem to give faster performance to worse local minima.

Convolutional Neural Networks





OME - MENU - CONNECT			T	'HE LATEST	POPULAR	MOST SHARED
MIT Technology Review	AKTHROUGH Ologies 201	3	Introduction	The 10 T	echnologies	Past Years
Deep Learning	Temporary Social Media	Prenatal DNA Sequencing	Additive Manufacturi	ing	Baxter: Collar R	The Blue- tobot
With massive amounts of computational power, machines can now recognize objects and translate speech in real time. Artificial intelligence is finally getting smart. →	Messages that quickly self-destruct could enhance the privacy of online communications and make people freer to be spontaneous.	Reading the DNA of fetuses will be the next frontier of the genomic revolution. But do you really want to know about the genetic problems or musical aptitude of your unborn child? →	Skeptical abou printing? GE, t world's larges manufacturer, the verge of u technology to parts.	ut 3-D the t is on sing the make jet →	Rodney I newest o easy to ir but the c innovatio robot she hard it is with peo	Brooks's creation is nteract with, omplex ns behind the ow just how to get along ple. →
Memory Implants	Smart Watches	Ultra-Efficient Solar	Big Data from		Supera	ride

(Unrelated) Dog vs Food





[Karen Zack, @teenybiscuit]

(Unrelated) Dog vs Food





[Karen Zack, @teenybiscuit]

CNNs in 2012: "SuperVision" (aka "AlexNet")

"AlexNet" — Won the ILSVRC2012 Challenge



Figure 2: An illustration of the architecture of our CNN, explicitly showing the delineation of responsibilities between the two GPUs. One GPU runs the layer-parts at the top of the figure while the other runs the layer-parts at the bottom. The GPUs communicate only at certain layers. The network's input is 150,528-dimensional, and the number of neurons in the network's remaining layers is given by 253,440–186,624–64,896–64,896–43,264–4096–4096–1000.

[Krizhevsky, Sutskever, Hinton. NIPS 2012]

Recap: Before Deep Learning



Input Extract Concatenate into Linear Pixels Features a vector **x** Classifier

Figure: Karpathy 2016

The last layer of (most) CNNs are linear classifiers



Input	Perform everything with a big neural
Pixels	network, trained end-to-end

Key: perform enough processing so that by the time you get to the end of the network, the classes are linearly separable

ConvNets

They're just neural networks with 3D activations and weight sharing
What shape should the activations have?

$$x \to \text{Layer} \to h^{(1)} \to \text{Layer} \to h^{(2)} \to \dots \to f$$

- The input is an image, which is 3D (RGB channel, height, width)

What shape should the activations have?

$$x \to \text{Layer} \to h^{(1)} \to \text{Layer} \to h^{(2)} \to \dots \to f$$

- The input is an image, which is 3D (RGB channel, height, width)

- We could flatten it to a 1D vector, but then we lose structure

What shape should the activations have?

$$x \to \text{Layer} \to h^{(1)} \to \text{Layer} \to h^{(2)} \to \dots \to f$$

- The input is an image, which is 3D (RGB channel, height, width)

- We could flatten it to a 1D vector, but then we lose structure

- What about keeping everything in 3D?

ConvNets

They're just neural networks with 3D activations and weight sharing





All Neural Net activations arranged in 3 dimensions:



All Neural Net activations arranged in **3 dimensions:**



For example, a CIFAR-10 image is a 3x32x32 volume (3 depth — RGB channels, 32 height, 32 width)

1D Activations:



1D Activations:

3D Activations:







- The input is 3x32x32
- This neuron depends on a 3x5x5 chunk of the input
- The neuron also has a 3x5x5 set of weights and a bias (scalar)



Example: consider the region of the input " x^{r} "

With output neuron h^r



Example: consider the region of the input " x^{r} "

With output neuron h^r

Then the output is:

$$h^r = \sum_{ijk} x^r_{ijk} W_{ijk} + b$$



Example: consider the region of the input " x^{r} "

With output neuron h^r

Then the output is:

$$h^{r} = \sum_{ijk} x^{r}_{ijk} W_{ijk} + b$$

Sum over 3 axes







With 2 output neurons

$$h_{1}^{r} = \sum_{ijk} x_{ijk}^{r} W_{1ijk} + b_{1}$$

$$h_{2}^{r} = \sum_{ijk} x_{ijk}^{r} W_{2ijk} + b_{2}$$



With 2 output neurons

$$h_{1}^{r} = \sum_{ijk} x_{ijk}^{r} W_{1ijk} + b_{1}$$

$$h_{2}^{r} = \sum_{ijk} x_{ijk}^{r} W_{2ijk} + b_{2}$$





We can keep adding more outputs

These form a column in the output volume: [depth x 1 x 1]



We can keep adding more outputs

These form a column in the output volume: [depth x 1 x 1]



Now repeat this across the input



Now repeat this across the input

Weight sharing:

Each filter shares the same weights (but each depth index has its own set of weights)





With weight sharing, this is called **convolution**



With weight sharing, this is called **convolution**

Without weight sharing, this is called a **locally** connected layer



One set of weights gives one slice in the output

To get a 3D output of depth *D*, use *D* different filters

In practice, ConvNets use many filters (~64 to 1024)



One set of weights gives one slice in the output

To get a 3D output of depth *D*, use *D* different filters

In practice, ConvNets use many filters (~64 to 1024)

All together, the weights are **4** dimensional: (output depth, input depth, kernel height, kernel width)







Figure: Andrej Karpathy

