Lecture 7:

Training Neural Networks Part II

Subhransu Maji, Chuang Gan and TAs Some slides kindly provided by Fei-Fei Li, Jiajun Wu, Erik Learned-Miller Lecture 7 - 1 Sep. 26, 2023

Projects: Overview

- 1. Parts
 - a. Proposal: October 8
 - **b. Milestone: November 5**
 - c. Final write-up: Dec. 8 (Friday)
- 2. Can't use extension "late days" for these deadlines!!!

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Projects as a mini-conference

- 1. You will write a paper with your team.
 - a. A suggested format will make sure you cover the right kinds of topics.
- 2. Everyone will participate in "paper reviewing".
 - a. These will be highly structured so you know what to comment on.
- 3. Subhransu and I will grade all the final write-ups at the same time as the reviews. We will not use the review scores directly

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Project Proposal

The project proposal should be concise (200-400 words). Your proposal should contain:

- Who are the (1~2) group members? What will each person do? (This needs to be a separate detailed paragraph)
- If the project is shared with another class, which portion of the work will be counted for each class? (This needs to be a separate detailed paragraph)
- What is the problem that you will be investigating? Why is it interesting?
- What data will you use? If you are collecting new datasets, how do you plan to collect them?
- What method or algorithm are you proposing? If there are existing implementations, will you use them and how? How do you plan to improve or modify such implementations?
- What reading will you examine to provide context and background?
- How will you evaluate your results? Qualitatively, what kind of results do you expect (e.g. plots or figures)? Quantitatively, what kind of analysis will you use to evaluate and/or compare your results (e.g. what performance metrics or statistical tests)?

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Submission: Please upload a PDF file named <your ID>_proposal.pdf to Gradescope. One submission for each group is sufficient.

Project Ideas

TA will give presentations on Oct. 3 (Next Tuesday)!!

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Overview

1. One time setup

activation functions, preprocessing, weight initialization, regularization, gradient checking

1. Training dynamics

babysitting the learning process, parameter updates, hyperparameter optimization

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1. Evaluation

model ensembles

Finish non-linearities from last time...

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Activation Functions



Sigmoid

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

- Squashes numbers to range [0,1]
- Historically popular since they have nice interpretation as a saturating "firing rate" of a neuron

2 problems:

- Saturated neurons "kill" the gradients
- 2. exp() is a bit compute expensive

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Activation Functions





- Does not saturate (in +region)
- Very little computation
- Converges much faster than sigmoid/tanh in practice (e.g. 6x)

ReLU (Rectified Linear Unit)

[Krizhevsky et al., 2012]

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What happens when x = -10? What happens when x = 0? What happens when x = 10?

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Activation Functions



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- Does not saturate
- Computationally efficient
- Converges much faster than sigmoid/tanh in practice! (e.g. 6x)
 will not "die".

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Leaky ReLU
$$f(x) = \max(0.01x, x)$$

Maxout "Neuron"

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- Generalizes ReLU and Leaky ReLU
- Linear Regime! Does not saturate! Does not die!

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

Problem: doubles the number of parameters/neuron :(

TLDR: In practice:

- Use ReLU. Be careful with your learning rates

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- Try out Leaky ReLU / Maxout
- Try out tanh but don't expect much
- Don't use sigmoid

Data Preprocessing

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Step 1: Preprocess the data



(Assume X [NxD] is data matrix, each example in a row)

Invariance of units

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Step 1: Preprocess the data



(Assume X [NxD] is data matrix, each example in a row)

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Preprocessing: Why are we doing this?

- Subtracting off the mean

- Avoid gradients that only point in two different orthants.

- Normalizing the magnitude

- Kilometers vs. millimeters...
 - Invariance to the specific *units* of the inputs...

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Step 1: Preprocess the data

In practice, you may also see **PCA** and **Whitening** of the data



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In practice for Images: center only

e.g. consider CIFAR-10 example with [32,32,3] images

- Subtract the mean image (e.g. AlexNet) (mean image = [32,32,3] array)
- Subtract per-channel mean (e.g. VGGNet) (mean along each channel = 3 numbers)

Not common to normalize variance, to do PCA or whitening

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Weight Initialization

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- Q: what happens when W=0 init is used?



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- First idea: **Small random numbers** (Gaussian with zero mean and 1e-2 standard deviation)

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- First idea: **Small random numbers** (Gaussian with zero mean and 1e-2 standard deviation)

$$W = 0.01^*$$
 np.random.randn(D,H)

Works ~okay for small networks, but can lead to non-homogeneous distributions of activations across the layers of a network.

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Let's look at some activation statistics

E.g. 10-layer net with 500 neurons on each layer, using tanh nonlinearities, and initializing as described in last slide.

```
# assume some unit gaussian 10-D input data
D = np.random.randn(1000, 500)
hidden_layer_sizes = [500]*10
nonlinearities = ['tanh']*len(hidden_layer_sizes)
```

```
act = {'relu':lambda x:np.maximum(0,x), 'tanh':lambda x:np.tanh(x)}
Hs = {}
for i in xrange(len(hidden_layer_sizes)):
    X = D if i == 0 else Hs[i-1] # input at this layer
    fan_in = X.shape[1]
    fan_out = hidden_layer_sizes[i]
    W = np.random.randn(fan_in, fan_out) * 0.01 # layer initialization
```

```
H = np.dot(X, W) # matrix multiply
H = act[nonlinearities[i]](H) # nonlinearity
Hs[i] = H # cache result on this layer
```

```
# look at distributions at each layer
print 'input layer had mean %f and std %f' % (np.mean(D), np.std(D))
layer means = [np.mean(H) for i,H in Hs.iteritems()]
layer_stds = [np.std(H) for i,H in Hs.iteritems()]
for i,H in Hs.iteritems():
    print 'hidden layer %d had mean %f and std %f' % (i+1, layer means[i], layer stds[i])
```

```
# plot the means and standard deviations
plt.figure()
plt.subplot(121)
plt.plot(Hs.keys(), layer_means, 'ob-')
plt.title('layer mean')
plt.subplot(122)
plt.plot(Hs.keys(), layer_stds, 'or-')
plt.title('layer std')
```

```
# plot the raw distributions
plt.figure()
for i,H in Hs.iteritems():
    plt.subplot(1,len(Hs),i+1)
    plt.hist(H.ravel(), 30, range=(-1,1))
```

```
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```

input layer had mean 0.000927 and std 0.998388 hidden layer 1 had mean -0.000117 and std 0.213081 hidden layer 2 had mean -0.000001 and std 0.047551 hidden layer 3 had mean -0.000002 and std 0.010630 hidden layer 4 had mean 0.000001 and std 0.002378 hidden layer 5 had mean 0.000002 and std 0.000532 hidden layer 6 had mean -0.000000 and std 0.000119 hidden layer 7 had mean 0.000000 and std 0.000026 hidden layer 8 had mean -0.000000 and std 0.000006 hidden layer 9 had mean 0.000000 and std 0.000001 hidden layer 10 had mean -0.000000 and std 0.000000



input layer had mean 0.000927 and std 0.998388 hidden layer 1 had mean -0.000117 and std 0.213081 hidden layer 2 had mean -0.000001 and std 0.047551 hidden layer 3 had mean -0.000002 and std 0.010630 hidden layer 4 had mean 0.000001 and std 0.002378 hidden layer 5 had mean 0.000002 and std 0.000532 hidden layer 6 had mean -0.000000 and std 0.000019 hidden layer 7 had mean 0.000000 and std 0.000026 hidden layer 8 had mean -0.000000 and std 0.000006 hidden layer 9 had mean 0.000000 and std 0.000006 hidden layer 10 had mean -0.000000 and std 0.000000



All activations become zero!

Q: think about the backward pass. What do the gradients look like?

Hint: think about backward pass for a W*X gate.

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W = np.random.randn(fan in, fan out) * 1.0 # layer initialization

input layer had mean 0.001800 and std 1.001311 hidden layer 1 had mean -0.000430 and std 0.981879 hidden layer 2 had mean -0.000849 and std 0.981649 hidden layer 3 had mean 0.000566 and std 0.981651 hidden layer 4 had mean 0.000483 and std 0.981755 hidden layer 5 had mean -0.000682 and std 0.981614 hidden layer 7 had mean -0.000401 and std 0.981560 hidden layer 7 had mean -0.000448 and std 0.981520 hidden layer 8 had mean -0.000448 and std 0.981913 hidden layer 9 had mean -0.000899 and std 0.981728 hidden layer 10 had mean 0.000584 and std 0.981736

*1.0 instead of *0.01



Almost all neurons completely saturated, either -1 and 1. Gradients will be all zero.

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input layer had mean 0.001800 and std 1.001311 hidden layer 1 had mean 0.001198 and std 0.627953 hidden layer 2 had mean 0.000175 and std 0.486051 hidden layer 3 had mean 0.000055 and std 0.486051 hidden layer 4 had mean 0.000142 and std 0.357108 hidden layer 5 had mean 0.000142 and std 0.320917 hidden layer 6 had mean -0.000389 and std 0.292116 hidden layer 7 had mean -0.000288 and std 0.273387 hidden layer 8 had mean -0.000291 and std 0.254935 hidden layer 9 had mean 0.000143 and std 0.239266 hidden layer 10 had mean 0.000139 and std 0.228008

0.0010

0.0008

0.0006

0.0004

0.0002

0.0000

-0.0002

-0.0004

20000

layer mean

layer std

"Xavier initialization" [Glorot et al., 2010]

Reasonable initialization. (Mathematical derivation assumes linear activations)

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300

0.60

0.55

0.50

0.45

0.40

0.35

0.30

0.25

Proper initialization is an active area of research...

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

Exact solutions to the nonlinear dynamics of learning in deep linear neural networks by Saxe et al, 2013

Random walk initialization for training very deep feedforward networks by Sussillo and Abbott, 2014

Delving deep into rectifiers: Surpassing human-level performance on ImageNet classification by He et al., 2015

Data-dependent Initializations of Convolutional Neural Networks by Krähenbühl et al., 2015

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All you need is a good init, Mishkin and Matas, 2015

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. . .

[loffe and Szegedy, 2015]



Usually inserted after Fully Connected / (or Convolutional, as we'll see soon) layers, and before nonlinearity.

$$\widehat{x}^{(k)} = \frac{x^{(k)} - \mathbf{E}[x^{(k)}]}{\sqrt{\operatorname{Var}[x^{(k)}]}}$$

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[loffe and Szegedy, 2015]

"you want unit Gaussian activations? just make them so." Not actually "Gaussian". Just zero mean, unit variance.

consider a batch of activations at some layer. To make each dimension unit normalized, apply:

$$\widehat{x}^{(k)} = \frac{x^{(k)} - \mathbf{E}[x^{(k)}]}{\sqrt{\operatorname{Var}[x^{(k)}]}}$$

this is a vanilla differentiable function...

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[loffe and Szegedy, 2015]

"you want unit Gaussian activations? just make them so." (you want NORMALIZED activations)



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[loffe and Szegedy, 2015]



Usually inserted after Fully Connected / (or Convolutional, as we'll see soon) layers, and before nonlinearity.

$$\widehat{x}^{(k)} = \frac{x^{(k)} - \mathbf{E}[x^{(k)}]}{\sqrt{\operatorname{Var}[x^{(k)}]}}$$

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[loffe and Szegedy, 2015]

Normalize:

$$\widehat{x}^{(k)} = \frac{x^{(k)} - \mathbb{E}[x^{(k)}]}{\sqrt{\operatorname{Var}[x^{(k)}]}}$$

And then allow the network to squash the range if it wants to:

$$y^{(k)} = \gamma^{(k)} \widehat{x}^{(k)} + \beta^{(k)}$$

Note, the network can learn: $\gamma^{(k)} = \sqrt{\text{Var}[x^{(k)}]}$ $\beta^{(k)} = \text{E}[x^{(k)}]$ to recover the identity mapping.

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[loffe and Szegedy, 2015]

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

 Improves gradient flow through the network

- Allows higher learning rates
- Reduces the strong dependence on initialization
- Acts as a form of regularization in a funny way, and slightly reduces the need for dropout, maybe

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[loffe and Szegedy, 2015]

Input: Values of x over a mini-b Parameters to be learned: Output: $\{y_i = BN_{\gamma,\beta}(x_i)\}$	atch: $\mathcal{B} = \{x_{1m}\};$ γ, β	Note: at test time BatchNorm layer functions differently:
$\mu_{\mathcal{B}} \leftarrow \frac{1}{m} \sum_{i=1}^{m} x_i$	// mini-batch mean	The mean/std are not computed based on the batch. Instead, a single fixed empirical mean of activations
$\sigma_{\mathcal{B}}^2 \leftarrow \frac{1}{m} \sum_{i=1}^m (x_i - \mu_{\mathcal{B}})^2$	// mini-batch variance	during training is used.
$\widehat{x}_i \leftarrow \frac{x_i - \mu_{\mathcal{B}}}{\sqrt{\sigma_{\mathcal{B}}^2 + \epsilon}}$	// normalize	(e.g. can be estimated during training with running averages)
$y_i \leftarrow \gamma \widehat{x}_i + \beta \equiv \mathbf{BN}_{\gamma,\beta}(x_i)$	// scale and shift	

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