### Machine Intelligence:: Deep Learning Week 3

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# Organizational Issues: Projects

- Projects (2-3 People)
- Presented on the last day
  - Spotlight talk (5 Minutes)
  - Poster
- Topics
  - You can choose a topic of your own (have to be discussed with us latest by week4 week5)
  - Possible Topics
    - Take part in a Kaggle Competition (e.g. Leaf Classification / Dogs vs. Cats)
    - Overview of google ml learning cloud for deep learning
    - Datasets e.g. http://www.vision.ee.ethz.ch/en/datasets/

- Please talk to us until week  $4 \rightarrow 5$
- Q&A Session 1h in week 7

# Organizational Issues: Times

- Next times (total 30 minutes break in between, possible different breaks)
  - 09:10 10:30 (We start 10 past 9)
  - 11:00 12:40
- Please interrupt us if something is unclear!

# Learning Objectives



- Increase our knowledge in TF
- Foundations of DL
  - Loss Function (what to minimize)
    - Cross entropy loss for multinomial logistic regression
    - Two principles to construct loss functions
      - Maximum Likelihood Principle
      - Cross Entropy
  - Deep Neural Networks
    - Fully Connected Networks with hidden layers
  - Gradient Descent
    - How to calculate the weights efficiently

# **Biological Interpretation**



• In popular media neural networks are often described as a computer model of the human brain.



Biological neurons are much more complicated.

Images from: http://cs231n.github.io/neural-networks-1/

# **Multinomial Logistic Regression**

# Multinomial logistic regression

- Logistic Regression outputs prob. for class 1
  - So far we can classify into two classes
- We now want to classify more than 2 classes

# Exercise: The MNIST Data Set

- MNIST the drosophila of all DL-Data sets
  - 50000 handwritten digits to be classified into 10 classes (0-9)



**Input tensors**: are flattened to 28\*28=768 pixels

# **Multinomial Logistic Regression**



# **Multinominal Regression**



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Multinomial case: just another **non-linearity** softmax  $p_1 = P(Y_1 = 1 | X = x) = \frac{\exp(\sum_i x_i W_{i1} + b_1)}{\sum_i \exp(\sum_i x_i W_{ij} + b_j)} = \operatorname{softmax}(\sum_i x_i W_{i1} + b_1)$ 

## Recap: Matrix Multiplication aka dot-product of matrices

We can only multiply matrices if their dimensions are compatible.

 $\mathbf{A} \times \mathbf{B} = \mathbf{C}$  $(\mathbf{m} \times \mathbf{n}) \times (\mathbf{n} \times \mathbf{p}) = (\mathbf{m} \times \mathbf{p})$ 

$$c_{11} = a_{11}b_{11} + a_{12}b_{21} + a_{13}b_{31}$$
  

$$c_{12} = a_{11}b_{12} + a_{12}b_{22} + a_{13}b_{32}$$
  

$$c_{21} = a_{21}b_{11} + a_{22}b_{21} + a_{23}b_{31}$$
  

$$c_{22} = a_{21}b_{12} + a_{22}b_{22} + a_{23}b_{32}$$
  

$$c_{31} = a_{31}b_{11} + a_{32}b_{21} + a_{33}b_{31}$$
  

$$c_{32} = a_{31}b_{12} + a_{32}b_{22} + a_{33}b_{32}$$

Example:

$$\mathbf{A}_{1x2} = \begin{pmatrix} 0 & 3 \end{pmatrix} \qquad \mathbf{B}_{2x3} = \begin{pmatrix} 3 & 1 & 7 \\ 8 & 2 & 4 \end{pmatrix} \qquad \mathbf{C}_{1x3} = \mathbf{A}_{1x2} \cdot \mathbf{B}_{2x3} = \begin{pmatrix} 24 & 6 & 12 \end{pmatrix}$$

# GPUs love matrices (or tensors)





$$(P_{1}, P_{1}) = Softmax \left( X_{1}W_{11} + X_{2}W_{21} + S_{1}, X_{4}W_{12} + X_{2}U_{21} + S_{2} \right)$$

$$= Softmax((X_{1}, X_{2})\begin{pmatrix} W_{1} & W_{12} \\ W_{21} & W_{22} \end{pmatrix} + (S_{1}, S_{2}))$$

$$P = Softmax(XW + 5)$$

$$p_{1} = P(Y_{1} = 1 | X = x) = \frac{\exp(\sum_{i} x_{i} W_{i1} + b_{1})}{\sum_{j} \exp(\sum_{i} x_{j} W_{ij} + b_{j})} = \operatorname{softmax}(\sum_{i} x_{i} W_{i1} + b_{1})$$

# Your turn

• Input x = (1,2)

• W = 
$$\begin{pmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \end{pmatrix}$$

- b = (1,2,3)
- Calculate the output using numpy:
- Hints:
- x = np.asarray([[1,2]]) #
- np.matmul(.,.) # Matrix multiplication
- np.exp(.) # Exponential
- np.sum(.) # Sum
- #Result: array([[3.29320439e-04, 1.79802867e-02, 9.81690393e-01]])





# GPUs love matrices: Use the source luke

Mini batch size at runtime

...

y = tf.nn.softmax(tf.matmul(x, W) + b)

Data is usually processed in (mini-) batches. Instead of X being a 28\*28=784 long vector, we use a batch (e.g. size 100)



## **GPUs love matrices:**



y = tf.nn.softmax(tf.matmul(x, W) + b)

Slide Credit: Martin Gröner TensorFlow and DL without a PhD https://docs.google.com/presentation/d/11/vew6ltsZ8igb6U17topeFit.SetHWOmMOwlgOY9co/pub?slde=id\_g110257a6da\_0\_4316

## Loss for multinomial regression

This is the prob. the model evaluates for the true class  $y^{(i)}$  of training example  $x^{(i)}$ 

Training Examples Y=1  
or Y=0
$$\lim_{x \to w^{(i)}} \lim_{x \to w^{(i)}$$

N Training Examples classes (1,2,3,...,K)

$$loss = -\frac{1}{N} \sum_{n=1}^{N} log(p_{model}(y^{(i)} | x^{(i)}; \theta)) = -\frac{1}{N} \left( \sum_{i \in y_j=1} log(p_1(x^{(i)})) + \sum_{i \in y_j=2} log(p_2(x^{(i)})) + \dots + \sum_{i \in y_j=K} log(p_K(x^{(i)})) \right)$$



Output of last layer

Example: Look at class of single training example. Say it's Dejan, if classified correctly  $p_{dejan} = 1 \rightarrow Loss = 0$ . Real bad classifier put's  $p_{dejan} = 0 \rightarrow Loss = Inf$ .

# One more Trick: Loss function with indicator function

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A one-hot-encoded y picks the right class, form all of the K different classes.

For MNIST K=10, so why calculate, 9 logs and through them away? (Parallel executions)

$$-N \cdot \log s = \sum_{i \in y_j = 1}^{N} \log(p_1(x^{(i)})) + \sum_{i \in y_j = 2}^{N} \log(p_2(x^{(i)})) + \dots + \sum_{i \in y_j = K}^{N} \log(p_K(x^{(i)})) = \sum_{i=1}^{N} y^{(i)} \log(p(x^{(i)})) = \sum_{i=1}$$

See later crossentropy and KL-Distance between  $y_i$  and  $p(x^{(i)})$ 

# Training Neural Networks: Split of the data

For neural networks usually no cross-validation is done (due to long learning times).

For our use case (4000 images)

- Training set 3000, Test set 1000
- 20% of the Training set is taken as Validation Set



same validation set.

# Stochastic gradient descent

• The loss function

$$loss = -\frac{1}{N} \sum_{n=1}^{N} log(p_{model}(y^{(i)} | x^{(i)}; \theta))$$



- A particular weight is updated using the partial derivative of the loss function (the sum) w.r.t  $\theta_i$
- The sum is taken over the whole training set of size N. Often the training set is split into mini-batches size of e.g. bs=128 (\*)
- These mini-batches are processed one after another
- When all examples have been processed once, we speak of one epoch being finished
- For a new epoch one often reshuffles the data
- The batch size is chosen so that input tensor fits on the GPU.

(\*) For some purists only when bs=1 is called stochastic gradient descent

# Exercise: The MNIST Data Set



#### Input tensors

One minibatch has dimension (128, 28, 28, 1) (batch, x,y, color)

or (128, 784) flattened

Image credit: https://www.tensorflow.org/versions/r0.10/images/MNIST-Matrix.png

# Exercise: Implement multinomial logistic regression

Finish the code in the notebook: Multinomial Logistic Regression

- Think about the trick how the loss is calculated!
- Compare the loss and accuracy in the validation set with the loss in the training set.
   Why is there such a difference?
- Question: How many parameters do we have?

#### Hints:



$$p_{j} = \frac{\exp(\sum_{i} x_{i} W_{ij} + b_{j})}{\sum_{j} \exp(\overline{\sum}_{i} x_{i} W_{ij} + b_{j})} = (\operatorname{softmax}(xW+b))_{j}$$



# SOLUTION

- We have
  - For W 28\*28\*10 = 7840 Parameter
  - For b 10 Parameter
  - Together 7850 Parameters



- Trick with the loss function [Blackboard]
  - loss = tf.reduce\_mean(-tf.reduce\_sum(y\_true \* tf.log(y\_pred), reduction\_indices=[1]))
- See:

https://github.com/tensorchiefs/dl course/blob/master/notebooks
/05 Multinomial Logistic Regression solution.ipynb

<u>https://github.com/tensorchiefs/dl\_course/blob/master/notebooks\_misc/Explanation\_c</u>
 <u>f\_loss.ipynb</u>

## Alternative solution

```
#Old Solution
prob = tf.nn.softmax(z)
loss_old = tf.reduce_mean(-tf.reduce_sum(y_true * tf.log(prob),
reduction_indices=[1]))
```

For numerical stability, one should use tf.nn.softmax\_cross\_entropy\_with\_logits

There is also a sparse version (no one hot encoded needed) tf.nn.sparse\_softmax\_cross\_entropy\_with\_logits

# Now we are well prepared to entre the realm of deep learning



# DEEPER

memegene



# Networks with hidden layers

# Limitations of (multinomial) logistics regression

Logistic regression in NN speak: "no hidden layer"



# Neural Network with hidden units

 Go to <u>http://playground.tensorflow.org</u> (https://goo.gl/VR3db5) and train a neural network for the data:



- Start with 0 hidden layers. Increase the number of hidden layers to one, what do you observe?
- Now go to <u>here</u> (https://goo.gl/XwLRKB) and increase the number of neurons in the hidden layer. What do you observe?



# Results

- 0 hidden layers, only a single line
- Many neurons in a hidden layer  $\rightarrow$  also complicated functions



# Results (cont)





# One hidden Layer



#### A network with one hidden layer is a universal function approximator!



http://cs231n.github.io/neural-networks-1/

# Brief History of Machine Learning (supervised learning)



With 1 hidden layer

# Examples of deep architectures



Original Resnet had 152 Layers: https://arxiv.org/abs/1512.03385

# Why going deep: Experimental evidence



The test set accuracy consistently increases with increasing depth. Just increasing model size does not yield the same performance.

Taken from: http://www.deeplearningbook.org/contents/mlp.html

# Why Deep: Hierarchy of learned features in Object Detection


## Why deeper (summary)?

- If a network with one hidden layer is a universal function approximator, why bother to go deeper?
  - Step functions are universal function approximators, too. Would you use them?
- Representational power:
  - There is experimental evidence that a 3 layered network needs less weights in total than a network with one hidden layer.
  - Theoretically backed for some functions
- For some applications as image classification there is a natural hierarchy of features to be learned
- More details see: <u>http://cs231n.github.io/neural-networks-1/#power</u> and references therein.
- Still active research area and not solved yet
  - Novel approach Tishby information plane, see e.g. his talk at Yandex <u>https://www.youtube.com/watch?v=bLqJHjXihK8</u>

### More than one layer

We have all the building blocks

- Use outputs as new inputs
- At the end use multin. logistic regression
- Names:
  - Fully connected network
  - Multi Layer Perceptron (MLP)





#### Summary

#### Softmax in last layer



### A network for classifying digits



#### Results



We get an accuracy of about 89% on the validation set.

Training error and loss approach zero. Validation error and loss increase with time (overfitting).

#### Summary

- Where do we stand?
  - In Principle we now can use deep networks
  - There are some tricks, we learn shortly.
  - To understand those tricks we have to get an understanding how learning works...

- Learning / gradient flow
  - Nowadays networks are learnt with gradient descent
  - For each weight a gradient w.r.t. loss is calculated and the weights are adapted
  - As we see a gradient signal flows from the loss to the input

#### Layer / chain structure of networks



#### Simple chaining

 $p = \text{softmax}(b^{(3)} + W^{(3)}f(b^{(2)} + W^{(2)}f(b^{(1)} + W^{(1)}x^{(1)})))$ 

# Backpropagation

Slide Credit to Elvis Murina for the great animations

#### Motivation: The forward and the backward pass

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https://google-developers.appspot.com/machine-learning/crash-course/backprop-scroll/



#### Chain rule recap

- If we have two functions f,g y = f(x) and z = g(y)then y and z are dependent variables.
- And by the chain rule:

$$\frac{\partial z}{\partial x} = \frac{\partial y}{\partial x} + \frac{\partial z}{\partial y}$$



#### Gradient flow in a computational graph: local junction



Illustration: http://cs231n.stanford.edu/slides/winter1516\_lecture4.pdf

### Example

$$f(x, y, z) = (x + y)z$$
  
e.g. x = -2. y = 5. z = -4







→ Multiplication do a switch

#### Forward pass



#### **Backward pass**



#### Forward pass



#### Side remark:

$$y = f(x)$$

$$g$$

$$z = g(y)$$

$$\dots$$

$$loss$$

$$\frac{\partial h}{\partial z}$$

- Some DL frameworks (e.g. Torch) do not do symbolic differentiation.
   For these for each operation needs to store only
  - The actual value y coming in and the value of derivative  $\frac{\partial g}{\partial y}|_{y}$



#### Further References / Summary

- For a more in depth treatment have a look at
  - Lecture 4 of <u>http://cs231n.stanford.edu/</u>
  - Slides <u>http://cs231n.stanford.edu/slides/winter1516\_lecture4.pdf</u>
- Gradient flow is important for learning: remember!



# Tricks of the trade



# **Activation Functions**

### Backpropagation through sigmoid



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

Gradients are killed, when not in active region! Slow learning!

#### Different activations in inner layers





Figure 1: A four-layer convolutional neural network with ReLUs (solid line) reaches a 25% training error rate on CIFAR-10 six times faster than an equivalent network with tanh neurons Source: Alexnet Krizhevsky et al 2012 There are other alternatives besides sigmoid and ReLU.

Currently ReLU is standard

#### Backpropagation through ReLU



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

Gradients are killed, only when x < 0

#### An activation which never gets killed...

• Why just don't take identity?



#### Other activations

# **Activation Functions**



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

[Mass et al., 2013] [He et al., 2015]

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

# Parametric Rectifier (PReLU)

 $f(x) = \max(\alpha x, x)$ 

backprop into \alpha (parameter)

Not really established

# Initialization

### Initialization of weights: Experiment

Layer (type)	Output	Shape	Param #	Connected to
dense_1 (Dense)	(None,	100)	78500	dense_input_1[0][0]
dense_2 (Dense)	(None,	100)	10100	dense_1[0][0]
dense_3 (Dense)	(None,	100)	10100	dense_2[0][0]
dense_4 (Dense)	(None,	100)	10100	dense_3[0][0]
dense_5 (Dense)	(None,	100)	10100	dense_4[0][0]
dense_6 (Dense)	(None,	100)	10100	dense_5[0][0]
dense_7 (Dense)	(None,	100)	10100	dense_6[0][0]
dense_8 (Dense)	(None,	100)	10100	dense_7[0][0]
dense_9 (Dense)	(None,	100)	10100	dense_8[0][0]
dense_10 (Dense)	(None,	10)	1010	dense_9[0][0]
Total parame: 160.310				
Trainable params: 160,310				
Non-trainable params: 0				

#### Weights are initialized with N(0, sigma)

See: <u>https://github.com/tensorchiefs/dl\_course/blob/master/notesbooks\_misc/weight\_initialization.ipynb</u>

### Different Initialization: Performance

Name	Smoothed
al estrelu_0.001	0.1067
🔵 relu_0.01	0.1233
🔵 relu_0.1	0.8855
🔵 relu_1.0	0.1017
elu_10	0.09000

val\_acc



Name	Smoothed
al etc.crelu_0.001	2.300
🔵 relu_0.01	2.300
v_arelu_0.1	0.01836
_ relu_1.0	14.57
<b>relu_10</b>	14.48



Learning happens only for sigma=0.1! Random loss is  $-\ln(1/10)=2.302$ 

#### Reason for not learning

- Activation values vanished or explode
- No learning since gradient is also vanishing
  - Grad ~ x and thus also near 0

- Historical anecdote
  - Deep Learning started 2006 when Hinton et. all managed to train deep networks unsupervised pre-training
  - Later it turned out that random initialization with the same weight would yield similar results
- For ReLU: He et al., http://arxiv.org/abs/1502.01852
  - sigma = np.sqrt(2. / fan\_in)
  - fan\_in number of incomming weights (100 in our example)
  - bias to zero



### Regularisation

Having more parameters than examples  $\rightarrow$  overfitting becomes a real problem

Several solutions (selection, for complete treatment <u>DL-book</u> chapter 7)

- Early stopping
- Dropout
- Not covered today
  - Penalties on parameter norm (L1, L2 a.k.a. weight decay)
  - Parameter tying and sharing (in the next lectures)
    - Very powerful for special domains
      - Time signals → RNN
      - Image like data →CNN
  - Dataset Augmentation (in CNN lecture)
  - Semi-supervised learning (use unlabelled data)

## Early stopping

• Simply stop (or use the parameters of the network) when validation loss is minimal (hope for the best for the test-set)



- In practice
  - Needs a validation set not used to update the weights
  - Save model weights at different epochs (*checkpoints*)
  - Plot and decide which checkpoint to use (or continue training)

## Early stopping (intuition)

- Early stopping can be seen as a from of regularization
- The optimization procedure cannot explore the whole parameter space
- Cannot adopt too much on the training set

#### Dropout

- Dropout is a simple and relatively recent regularization technique (Srivastava et al. 2014) which is already widely used.
- It forces the network to learn redundant features
- It averages over many networks







(b) After applying dropout.

Figure: from paper

### Dropout: training / testing

- At test time we (usually) want deterministic predictions
  - Later in the course we use them to make stochastic predictions
- Weights (connections) need to be downweighted by p
  - During training the connections have not been present with prob. p, they would thus be too strong if always present in test time



- Alternative approach (inverted dropout)
  - Upweight the weights by W/p during training (see also: <u>http://cs231n.github.io/neural-networks-2/</u>)
  - No scaling needed at test-time

### Higher level libraries

- Including all the logging and regularisation would require to write lot of code
- There is a multitude of libraries (currently too many!) which help you with training and setting up the networks
- Libraries make use of the Lego like block structure of networks




# Have a look at

# https://github.com/tensorchief s/dl\_course\_2018/blob/master/ docs/keras-short-intro.pdf

#### **Example in Keras**

```
model = Sequential() #We start to build the model in a sequence
model.add(Dense(500, batch_input_shape=(None,
784),activity_regularizer=activity_l2(lambd)))
model.add(Dropout(0.5))
model.add(BatchNormalization())
model.add(Activation('relu'))
```

```
model.add(Dense(50,activity_regularizer=activity_l2(lambd)))
model.add(Dropout(0.5))
model.add(BatchNormalization())
model.add(Activation('relu'))
```



# Why the hack they call it cross entropy?

# Entropy and Cross Entropy

 The central loss function for classification is called cross entropy, why?



- This is a different viewpoint to the max-likelihood approach, we just had
- Let's start by defining the (information) entropy
  - It's somewhat like the amount of surprise you get from a sample.
  - Let's first do an simple example

## Information Content of a single outcome

• 4 Balls each with same probability 25%



• How can your friend ask you which ball you picked, with minimum number of questions?



Let's say we have a red ball. Two questions need to be ask.

Coding for red ball (yes=1) 10 // Information content 2 bits

Coding for orange (your turn) 00 // Information content 2 bits

# Information Content of a single outcome

• 4 Balls each with different probability 50%, 25%, 12.5%, 12.5%



• How can your friend ask you which ball you picked, with minimum number of questions (on average)?



Let's say we have a blue ball. One questions need to be ask.

Coding for blue ball (yes=1) 1 // Information content 1 bit

Coding for red (2 questions) 01 // Information content 2 bit

Coding for green (your turn) 001 // Information content 3 bit

#### Information content



On average: <sup>1</sup>/<sub>2</sub>\*1+1/4\*2+1/4\*3=1.75 bits on average

#### **Information Content**

- For that easy example, we found the best coding by hand.
- Let's define the (self-) information (Turns out to be the minimal coding length "Shannon's source coding theorem")
- Requirement for Information (or surpirse)
  - $p_i$  the probability of event i (or prob. that symbol i occurs)
  - Seldom examples should have more surprise.
    - $I(p_i)$  should be monotonic decreasing function
  - Information should be non-negative
    - $I(p_i) \ge 0$
  - Uninformative, or sure events should have no Information
    - $I(p_i) = 0$
  - Information of independent events *i*, *j* should add up
    - $I(p_{(i,j)}) = I(p_i p_j) = I(p_i) + I(p_j)$
- $\rightarrow I(p) = -\log_2(p)$ 
  - (defined up to basis), 2 is often chosen

# Information Content $\rightarrow$ Entropy

• Entropy (average Information Content)

 $- \qquad H(p) = \sum p_i I(p_i) = -\sum p_i \log_2(p_i)$ 



In general: Maximal Entropy if uniform, minimal if peaked (see also in physical Systems)

# **Cross Entropy**

- If we know the distribution p, we can find the best coding and need H bits on average
- If we have a "wrong" distribution q how many bits do we need on average

 $-H(p,q) = -\sum p_i \log 2(q_i) \ge H(p)$ 

• Example, we think symbols come uniform distributed q. But they come (0.5,0.25,0.125,0.125)



$$H(p,q) = 0.52 + 0.252 + 0.125 * 2 + 0.1252 = 2 > 1.75$$

Optimal Coding Scheme for Uniform q

#### **KL-Divergence**

• If we have a "wrong" distribution q how many bits do we have more than the minimal possible amount H(p)

 $- D_{KL}(p||q) = H(p,q) - H(p) \ge 0$ 

• Example, we think symbols come uniform distributed q. But they come (0.5,0.25,0.125,0.125)



$$D(p,q) = H(p,q) - H(p) = 2 - 1.75 = 0.25$$

Optimal Coding Scheme for Uniform q

# **Cross Entropy in DL**



 $H(p,q) = -\sum p_i lnq_i$  (for one example of the training set)

$$H(p,q) = -\sum p_i^{(j)} ln q_i^j$$
 (for the training set)

We minimize the cross entropy by changing q, the minimum is reached when q is identical to distribution of real labels p

Alternatively we could also minimize the KL-Divergence

#### Further Resources (cross entropy and information theory)

- <u>https://rdipietro.github.io/friendly-intro-to-cross-entropy-loss/</u>
- https://www.quora.com/Whats-an-intuitive-way-to-think-of-crossentropy
- https://www.khanacademy.org/computing/computerscience/informationtheory/moderninfotheory/v/information-entropy
- https://medium.com/swlh/shannon-entropy-in-the-context-ofmachine-learning-and-ai-24aee2709e32