DS 4400

Machine Learning and Data Mining I

Alina Oprea Associate Professor, CCIS Northeastern University

November 8 2018

Logistics

- HW 3 is due on Tuesday, November 13
- Project Milestone is due on Tuesday, November 20
- Class on November 27 is cancelled
- Final project presentations
 - Monday, December 3, 3-5:30pm in ISEC 655
- Final exam

– Tuesday, Dec 11, 2-5pm in ISEC 655

Review

- To train neural networks, need to decide first on architecture
 - Number of layers, number of hidden units, connections between neurons, activation functions
- Randomly initialize parameters
- For each training example, use forward propagation to compute prediction
- Use backpropagation to propagate the error from last layer back into the network

References

- Stanford tutorial on training Multi-Layer Neural Networks
 - <u>http://ufldl.stanford.edu/tutorial/supervised/Mult</u>
 <u>iLayerNeuralNetworks/</u>
- Notes on backpropagation by Andrew Ng
 - <u>http://cs229.stanford.edu/notes/cs229-notes-backprop.pdf</u>
- Deep learning notes by Andrew Ng
 - <u>http://cs229.stanford.edu/notes/cs229-notes-</u> <u>deep_learning.pdf</u>

Outline

- Training with backpropagation
 - Gradient-Descent Algorithm
 - Derivation of gradients
 - Stochastic and Mini-Batch Gradient Descent
- Lab
 - MNIST dataset
- Regularization for Neural Networks
 - L2/L1 regularization
 - Dropout

Forward Propagation

- The input neurons first receive the data features of the object. After processing the data, they send their output to the first hidden layer.
- The hidden layer processes this output and sends the results to the next hidden layer.
- This continues until the data reaches the final output layer, where the output value determines the object's classification.
- This entire process is known as Forward Propagation, or Forward prop.



Learning in NN: Backpropagation

- Similar to the perceptron learning algorithm, we cycle through our examples
 - If the output of the network is correct, no changes are made
 - If there is an error, weights are adjusted to reduce the error
- The trick is to assess the blame for the error and divide it among the contributing weights

Error at last layer can be measured, but it is challenging to determine error at intermediate hidden layers

GD for Neural Networks

Initialization

- For all layers ℓ
 - Set $W^{[\ell]}$, $b^{[\ell]}$ at random
- Backpropagation
 - Fix learning rate α
 - For all layers ℓ (starting backwards)

•
$$W^{[\ell]} = W^{[\ell]} - \alpha \sum_{i=1}^{N} \frac{\partial L(\hat{y}^{(i)}, y^{(i)})}{\partial W^{[\ell]}}$$

•
$$b^{[\ell]} = b^{[\ell]} - \alpha \sum_{i=1}^{N} \frac{\partial L(\hat{y}^{(i)}, y^{(i)})}{\partial b^{[\ell]}}$$

Example



Dimension d

$$\begin{split} z^{[1]} &= W^{[1]} x^{(i)} + b^{[1]} \\ a^{[1]} &= g(z^{[1]}) \\ z^{[2]} &= W^{[2]} a^{[1]} + b^{[2]} \\ a^{[2]} &= g(z^{[2]}) \\ z^{[3]} &= W^{[3]} a^{[2]} + b^{[3]} \\ \hat{y}^{(i)} &= a^{[3]} = g(z^{[3]}) \end{split}$$

Parameters are initialized with random values (not all 0)!

Backpropagation Intuition



$$\begin{split} \delta_{j}^{(l)} &= \text{``error'' of node } j \text{ in layer } l \\ \text{Formally, } \delta_{j}^{(l)} &= \frac{\partial}{\partial z_{j}^{(l)}} \text{cost } (x^{(i)}) \\ cost(x^{(i)}) &= y^{(i)} \log h_{\theta}(x^{(i)}) + (1 - y^{(i)}) \log(1 - h_{\theta}(x^{(i)})) \end{split}$$

Backpropagation Intuition



Backpropagation Intuition



Training

- Training data $x^{(1)}$, $y^{(1)}$, ... $x^{(N)}$, $y^{(N)}$
- One training example $x^{(i)} = (x_1^{(i)}, \dots, x_d^{(i)})$, label $y^{(i)}$
- One forward pass through the network – Compute prediction $\hat{y}^{(i)}$
- Loss function for one example

$$-L(\hat{y}, y) = -[(1-y)\log(1-\hat{y}) + y\log\hat{y}]$$

Cross-entropy loss

• Loss function for training data

$$-J(W,b) = \frac{1}{N} \sum_{i} L(\hat{y}^{(i)}, y^{(i)}) + \lambda R(W, b)$$

Backpropagation

Let $\delta_j^{(l)} =$ "error" of node j in layer l $L(y, \hat{y}) = -[(1 - y)\log(1 - \hat{y}) + y\log \hat{y}]$

• Definitions

$$- z^{[\ell]} = W^{[\ell]} a^{[\ell-1]} + b^{[\ell]}, a^{[\ell]} = g(z^{[\ell]})$$

$$-\delta^{[\ell]} = \frac{\partial L(\hat{y}, y)}{\partial z^{[\ell]}}$$



Example: Last Layer (3)

•
$$\delta^{[3]} = \frac{\partial L(\hat{y}, y)}{\partial z^{[3]}} = \frac{\partial L(\hat{y}, y)}{\partial \hat{y}} g'(z^{[3]}); \hat{y} = g(z^{[3]}) = a^{[3]}$$
•
$$\frac{\partial L(\hat{y}, y)}{\partial \hat{y}} = -\frac{\partial [(1-y)\log(1-\hat{y})+y\log\hat{y}]}{\partial \hat{y}} = \frac{1-y}{1-\hat{y}} - \frac{y}{\hat{y}} = \frac{\hat{y}-y}{\hat{y}(1-\hat{y})}$$
•
$$\delta^{[3]} = \frac{\hat{y}-y}{\hat{y}(1-\hat{y})} g'(z^{[3]})$$

$$= \frac{a^{[3]}-y}{g(z^{[3]})(1-g(z^{[3]}))} g(z^{[3]}) (1-g(z^{[3]})) = a^{[3]} - y$$
•
$$\frac{\partial L(\hat{y}, y)}{\partial W^{[3]}} = \delta^{[3]} a^{[2]T} = (a^{[3]} - y) a^{[2]T}$$

•
$$\frac{\partial L(\hat{y}, y)}{\partial b^{[3]}} = a^{[3]} - y$$

$$g(x) = \sigma(x) = \frac{1}{1 + e^{-x}}$$
$$g'(x) = \sigma'(x) = \sigma(x)(1 - \sigma(x))$$

Example: Layer 2

•
$$\delta^{[2]} = \frac{\partial L(\hat{y}, y)}{\partial z^{[2]}} = \delta^{[3]} W^{[3]} g'(z^{[2]})$$

•
$$\frac{\partial L(\hat{y}, y)}{\partial W^{[2]}} = \delta^{[2]} a^{[1]T} = \delta^{[3]} W^{[3]} g'(z^{[2]}) a^{[1]T} = [a^{[3]} - y] W^{[3]} g(z^{[2]}) (1 - g(z^{[2]})) a^{[1]T}$$

•
$$\frac{\partial L(\hat{y}, y)}{\partial b^{[2]}} = [a^{[3]} - y] W^{[3]} g(z^{[2]}) (1 - g(z^{[2]}))$$

$$g(x) = \sigma(x) = \frac{1}{1 + e^{-x}}$$
$$g'(x) = \sigma'(x) = \sigma(x)(1 - \sigma(x))$$

Batch Perceptron



- Simplest case: α = 1 and don't normalize, yields the fixed increment perceptron
- Each increment of outer loop is called an epoch

Backpropagation

Set $\Delta_{ij}^{(l)} = 0 \quad \forall l, i, j$ (Used to accumulate gradient) For each training instance $(x^{(i)}, y^{(i)})$ Set $\mathbf{a}^{(1)} = \mathbf{x}_i$ Compute $\{\mathbf{a}^{(2)}, \dots, \mathbf{a}^{(L)}\}$ via forward propagation Compute $\delta^{(L)} = \mathbf{a}^{(L)} - y^{(i)}$ Compute errors $\{\delta^{(L-1)}, \dots, \delta^{(2)}\}$ Compute gradients $\Delta_{ij}^{(l)} = \Delta_{ij}^{(l)} + a_j^{(l)} \delta_i^{(l+1)}$

Average gradient is
$$\frac{\Delta_{ij}^{[\ell]}}{N}$$

Training NN with Backpropagation

Given training set $(x_1, y_1), ..., (x_N, y_N)$ Initialize all parameters $W^{[\ell]}, b^{[\ell]}$ randomly, for all layers ℓ Loop

Set $\Delta_{ij}^{(l)} = 0 \quad \forall l, i, j$ (Used to accumulate gradient) For each training instance $(x^{(i)}, y^{(i)})$ Set $\mathbf{a}^{(1)} = \mathbf{x}_i$ Compute $\{\mathbf{a}^{(2)}, \dots, \mathbf{a}^{(L)}\}$ via forward propagation **EPOCH** Compute $\boldsymbol{\delta}^{(L)} = \mathbf{a}^{(L)} - y^{(i)}$ Compute errors $\{\boldsymbol{\delta}^{(L-1)}, \dots, \boldsymbol{\delta}^{(2)}\}$ Compute gradients $\Delta_{ij}^{(l)} = \Delta_{ij}^{(l)} + a_j^{(l)} \delta_i^{(l+1)}$

Update weights via gradient step

•
$$W_{ij}^{[\ell]} = W_{ij}^{[\ell]} - \alpha \frac{\Delta_{ij}^{[\ell]}}{N}$$

• Similar for $b_{ij}^{[\ell]}$

Until weights converge or maximum number of epochs is reached

GD for Neural Networks

Initialization

- For all layers ℓ
 - Set $W^{[\ell]}$, $b^{[\ell]}$ at random
- Backpropagation
 - Fix learning rate α
 - For all layers ℓ (starting backwards)

•
$$W^{[\ell]} = W^{[\ell]} - \alpha \sum_{i=1}^{N} \frac{\partial L(\hat{y}^{(i)}, y^{(i)})}{\partial W^{[\ell]}}$$

• $b^{[\ell]} = b^{[\ell]} - \alpha \sum_{i=1}^{N} \frac{\partial L(\hat{y}^{(i)}, y^{(i)})}{\partial b^{[\ell]}}$

This is expensive!

Stochastic Gradient Descent (SGD)

Initialization

- For all layers ℓ
 - Set $W^{[\ell]}$, $b^{[\ell]}$ at random
- Backpropagation
 - Fix learning rate α
 - For all layers ℓ (starting backwards)
 - For all training examples $x^{(i)}$, $y^{(i)}$

$$\begin{split} -W^{[\ell]} &= W^{[\ell]} - \alpha \frac{\partial L(\hat{y}^{(i)}, y^{(i)})}{\partial W^{[\ell]}} \\ -b^{[\ell]} &= b^{[\ell]} - \alpha \frac{\partial L(\hat{y}^{(i)}, y^{(i)})}{\partial b^{[\ell]}} \end{split}$$

Incremental version of GD

Mini-batch Gradient Descent

Initialization

- For all layers ℓ
 - Set $W^{[\ell]}$, $b^{[\ell]}$ at random
- Backpropagation
 - Fix learning rate α
 - For all layers ℓ (starting backwards)
 - For all batches b of size B with training examples $x^{(ib)}$, $y^{(ib)}$

$$-W^{[\ell]} = W^{[\ell]} - \alpha \sum_{i=1}^{B} \frac{\partial L(\hat{y}^{(ib)}, y^{(ib)})}{\partial W^{[\ell]}}$$
$$-b^{[\ell]} = b^{[\ell]} - \alpha \sum_{i=1}^{B} \frac{\partial L(\hat{y}^{(ib)}, y^{(ib)})}{\partial b^{[\ell]}}$$

Gradient Descent Variants



Gradient Descent Variants



- Batch gradient descent
- Mini-batch gradient Descent
- Stochastic gradient descent

Training Neural Networks

Pick a network architecture (connectivity pattern between nodes)







- # input units = # of features in dataset
- # output units = # classes

Reasonable default: 1 hidden layer

 or if >1 hidden layer, have same # hidden units in every layer (usually the more the better)

Training Neural Networks

- Randomly initialize weights
- Implement forward propagation to get prediction \hat{y}_i for any training instance x_i
- Compute loss function $L(\hat{y}_i, y_i)$
- Implement backpropagation to compute partial derivatives $\frac{\partial L(\hat{y}^{(i)}, y^{(i)})}{\partial W^{[\ell]}}$ and $\frac{\partial L(\hat{y}^{(i)}, y^{(i)})}{\partial b^{[\ell]}}$
- Use gradient descent with backpropagation to compute parameter values that optimize loss

MNIST: Handwritten digit recognition



Images are 28 x 28 pixels

Represent input image as a vector $\mathbf{x} \in \mathbb{R}^{784}$ Learn a classifier $f(\mathbf{x})$ such that, $f: \mathbf{x} \to \{0, 1, 2, 3, 4, 5, 6, 7, 8, 9\}$

> Predict the digit Multi-class classifier

Lab – Feed Forward NN

```
import time
import numpy as np
from keras.utils import np_utils
import keras.callbacks as cb
from keras.models import Sequential
from keras.layers.core import Dense, Dropout, Activation
from keras.optimizers import RMSprop
from keras.datasets import mnist
import matplotlib
```

```
matplotlib.use('agg')
import matplotlib.pyplot as plt
```

```
def load_data():
    print("Loading data")
    (X_train, y_train), (X_test, y_test) = mnist.load_data()
```

```
X_train = X_train.astype('float32')
X_test = X_test.astype('float32')
```

```
# Normalize
```

X_train /= 255 X_test /= 255

```
y_train = np_utils.to_categorical(y_train, 10)
y_test = np_utils.to_categorical(y_test, 10)
```

```
X_train = np.reshape(X_train, (60000, 784))
X_test = np.reshape(X_test, (10000, 784))
```

```
print("Data Loaded")
return [X_train, X_test, y_train, y_test]
```

Import modules

Load MNIST data

Define NN architecture



Train and evaluate

```
def run_network(data=None, model=None, epochs=20, batch=256):
    try:
        start_time = time.time()
        if data is None:
            X_train, X_test, y_train, y_test = load_data()
        else:
            X_train, X_test, y_train, y_test = data
                                                                             class LossHistory(cb.Callback):
         if model is None:
                                                                                 def on train begin(self, logs={}):
            model = init_model()
                                                                                     self.losses = []
        history = LossHistory()
                                                                                 def on_batch_end(self, batch, logs={}):
                                                                                     batch loss = logs.get('Loss')
        print("Training model")
                                                                                     self.losses.append(batch loss)
        model.fit(X_train, y_train, nb_epoch=epochs, batch_size=batch,
                   callbacks=[history],
                   validation_data=(X_test, y_test), verbose=2)
        print("Training duration:"+format(time.time() - start_time))
        score = model.evaluate(X test, y test, batch size=16)
        print("\nNetwork's test Loss and accuracy:"+format(score))
```

return model, history.losses

Run code

model, losses = run_network()

[alina@dome MNIST]\$ python3 ffnn.py Using TensorFlow backend. Loading data Data loaded Compiling Model WARNING:tensorflow:From /usr/local/lib/python3.6/site-packages/keras/backend/ten sorflow backend.py:2755: calling reduce sum (from tensorflow.python.ops.math ops with keep dims is deprecated and will be removed in a future version. Instructions for updating: keep dims is deprecated, use keepdims instead WARNING:tensorflow:From /usr/local/lib/python3.6/site-packages/keras/backend/ten sorflow backend.py:1290: calling reduce mean (from tensorflow.python.ops.math op s) with keep dims is deprecated and will be removed in a future version. Instructions for updating: keep dims is deprecated, use keepdims instead Model finished0.22017550468444824 Training model /usr/local/lib/python3.6/site-packages/keras/models.py:848: UserWarning: The `nb epoch' argument in 'fit' has been renamed 'epochs'. warnings.warn('The `nb epoch' argument in `fit` ' Train on 60000 samples, validate on 10000 samples

Epoch 1/20

2018-08-29 20:02:45.664799: I tensorflow/core/common runtime/qpu/qpu device.c name: TITAN X (Pascal) major: 6 minor: 1 memoryClockRate(GHz): 1.531 pciBusID: 0000:83:00.0 totalMemory: 11.90GiB freeMemory: 406.00MiB 2018-08-29 20:02:45.664916: I tensorflow/core/common runtime/gpu/gpu device.c 2018-08-29 20:02:46.044142: I tensorflow/core/common runtime/gpu/gpu device.c lica:0/task:0/device:GPU:0 with 127 MB memory) -> physical GPU (device: 0, na te capability: 6.1) 2s - loss: 0.3561 - acc: 0.8916 - val loss: 0.1441 - val acc: 0.9550 Epoch 2/20 1s - loss: 0.1545 - acc: 0.9538 - val loss: 0.0939 - val acc: 0.9706 Epoch 3/20 1s - loss: 0.1128 - acc: 0.9663 - val loss: 0.0796 - val acc: 0.9744 Epoch 4/20 1s - loss: 0.0923 - acc: 0.9718 - val loss: 0.0739 - val acc: 0.9767 Epoch 5/20 1s - loss: 0.0803 - acc: 0.9755 - val loss: 0.0792 - val acc: 0.9767 Epoch 6/20 1s - loss: 0.0722 - acc: 0.9782 - val loss: 0.0701 - val acc: 0.9800 Epoch 7/20 1s - loss: 0.0645 - acc: 0.9802 - val loss: 0.0720 - val acc: 0.9814 Epoch 8/20 1s - loss: 0.0590 - acc: 0.9824 - val loss: 0.0700 - val acc: 0.9811 Epoch 9/20 1s - loss: 0.0522 - acc: 0.9833 - val loss: 0.0723 - val acc: 0.9792 Epoch 10/20 1s - loss: 0.0522 - acc: 0.9844 - val loss: 0.0659 - val acc: 0.9826 Epoch 11/20 1s - loss: 0.0460 - acc: 0.9861 - val loss: 0.0646 - val acc: 0.9847 Epoch 12/20 1s - loss: 0.0442 - acc: 0.9867 - val loss: 0.0696 - val acc: 0.9825 Epoch 13/20 1s - loss: 0.0438 - acc: 0.9866 - val loss: 0.0731 - val acc: 0.9824 Epoch 14/20 1s - loss: 0.0396 - acc: 0.9881 - val loss: 0.0702 - val acc: 0.9837 Epoch 15/20 1s - loss: 0.0371 - acc: 0.9888 - val loss: 0.0822 - val acc: 0.9831 Epoch 16/20 1s - loss: 0.0372 - acc: 0.9887 - val loss: 0.0736 - val acc: 0.9837 Epoch 17/20 1s - loss: 0.0347 - acc: 0.9893 - val loss: 0.0755 - val acc: 0.9830 Epoch 18/20 1s - loss: 0.0323 - acc: 0.9901 - val loss: 0.0749 - val acc: 0.9839 Epoch 19/20 1s - loss: 0.0340 - acc: 0.9899 - val loss: 0.0754 - val acc: 0.9831 Epoch 20/20 Training duration:25.691107034683228 9568/10000 [=====>..] - ETA: 0s Network's test loss and accuracy:[0.083858822271390659, 0.9815000000000004]

Epoch Output

Metrics

- Loss
- Accuracy

Plot Batch Loss



Outline

- Training with backpropagation
 - Gradient-Descent Algorithm
 - Derivation of gradients
 - Stochastic and Mini-Batch Gradient Descent
- Lab
 - MNIST dataset
- Regularization for Neural Networks
 - L2/L1 regularization
 - Dropout

Overfitting



- The larger the network, the higher the capacity (more model parameters)
- But also more prone to overfitting!

Regularization





 λ = regularization strength (hyperparameter)

Data loss: Model predictions should match training data

Regularization: Prevent the model from doing too well on training data

L2 regularization: $R(W) = \sum_{k} \sum_{l} W_{k,l}^2$ Weight decay L1 regularization: $R(W) = \sum_k \sum_l |W_{k,l}|$ Elastic net (L1 + L2): $R(W) = \sum_{k} \sum_{l} \beta W_{k,l}^{2} + |W_{k,l}|$

When computing gradients of loss function, regularization term needs to be taken into account

Dropout



- Figure 1: Dropout Neural Net Model. Left: A standard neural net with 2 hidden layers. Right: An example of a thinned net produced by applying dropout to the network on the left. Crossed units have been dropped.
- Regularization technique that has proven very effective for deep learning
- Srivastava et al. Dropout: A Simple Way to Prevent Neural Networks from Overfitting. Journal of Machine Learning Research 15, 2014

Dropout



Figure 2: Left: A unit at training time that is present with probability p and is connected to units in the next layer with weights w. **Right**: At test time, the unit is always present and the weights are multiplied by p. The output at test time is same as the expected output at training time.

- At training time, sample a sub-network and learn weights
 - Keep each neuron with probability p
- At testing time, all neurons are there, but reduce weight by a factor of p

Dropout



Figure 3: Comparison of the basic operations of a standard and dropout network.

- $r_i^{(\ell)}$ Is a random variable taking value 1 with probability p and value 0 with probability 1-p
- Multiply output of each layer by $r_i^{(\ell)}$

Results on MNIST



Figure 4: Test error for different architectures with and without dropout. The networks have 2 to 4 hidden layers each with 1024 to 2048 units.

Hyper-parameter learning

• Architecture

- Number layers, hidden units, activation functions

- Regularization
- Learning rate

- Can tune hyper-parameters with crossvalidation
- More advanced techniques: meta learning

Acknowledgements

- Slides made using resources from:
 - Yann LeCun
 - Andrew Ng
 - Eric Eaton
 - David Sontag
 - Andrew Moore
- Thanks!