Software Packages for Deep Learning

Chensong Zhang

with Zheng Li and Ronghong Fan

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Outline

Introduction

Comparison

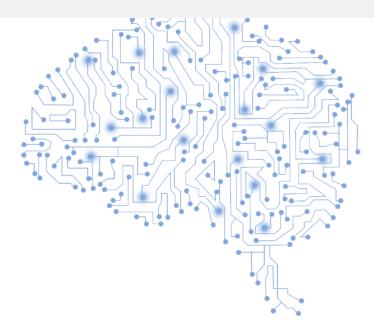
Python

TensorFlow

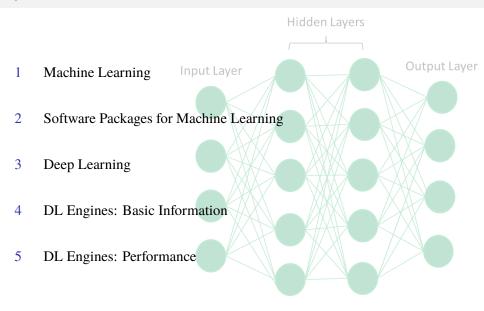
MXNet

Torch

Caffe



§1. Introduction



Machine Learning



Why ML now?

- Unlike traditional numerical simulation, "ML gives computers the ability to learn without being explicitly programmed" [Samuel 1959]
- As a research field, ML explores the study and construction of algorithms that can learn from and make predictions on data
- Fourth paradigm, big data, artificial intelligence, Internet of things, ...

General Tasks of ML:

- Classification: Inputs are divided into two or more classes, and the learner must produce a model that assigns unseen inputs to one or more (multi-label classification) of these classes
- Clustering: Inputs are divided into groups. Unlike in classification, the groups are not known beforehand, making this typically an unsupervised task
- Regression: Similar to classification, but the outputs are continuous
- Density estimation, dimensionality reduction, ...

Software Packages for Machine Learning

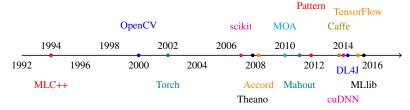


What is the purpose?

- Solving problems from practical applications (user interface)
- Developing algorithms and optimizing implementation (development)
- Theoretical analysis for machine learning

What do we want for a ML package?

- Easy for new tasks and new network structures (less steep learning curve)
- Easy for debugging (with good support and large community)
- Performance and scalability



Deep Learning



Deep Learning has been introduced with the objective of moving ML closer to one of its original goals—AI. The main motivations includes:

- Insufficient depth can hurt
- The brain has a deep architecture
- Cognitive processes seem deep

Pros:

- conceptually simple
- nonlinear
- highly flexible and configurable
- learned features can be extracted
- can be fine-tuned with more data
- efficient for multi-class problems
- world-class at pattern recognition

Cons:

- hard to interpret
- theory not well understood
- slow to train and score
- overfits, needs regularization
- more parameters
- inefficient for categorical variables
- data hungry, learns slowly

DL Engines: Basic Information



Viewpoint	Torch	Caffe	TensorFlow	MXNet	
Released	2002	2013	2015	2015	
Main Developers	Facebook, Twitter, Google,	BAIR BVLC	Google	DMLC C++	
Core Languages	C/Lua	C++	C++ Python		
Supported	Lua	C++/Python	C++/Python/R	C++/Python/R	
Interface	Lua	Matlab	Java/Go	Matlab/Julia/	
License	BSD	BSD	Apache	Apache	

- Other worth-noting's: CNTK/DMTK (Microsoft), Neon (Nervana & Intel), PyTorch (beta)
- BAIR, Berkeley Artificial Intelligence Research Lab
- BVLC, Berkeley Vision and Learning Center
- DMLC, Distributed (Deep) Machine Learning Community, supported by Amazon, Intel, Microsoft, nVidia, Baidu, ...

DL Engines: Performance



Viewpoint	Torch	Caffe	TensorFlow	MXNet
Pretrained Models	Yes	Yes No		Yes
High-level Support	Good	Good	Good	Good
Low-level Operators	Good	Good	Fairly good	Increasing fast
Speed One-GPU	Great	Great	Not so good	Excellent
Memory Management	Great	Great	Not so good	Excellent
Parallel Support	Multi-GPU	Multi-GPU	Multi-GPU	Distributed
Coding Style	Imperative	Imperative	Declarative	Declarative Imperative
GitHub Watching	649/268	1856	4939	887

§2. Comparison

Hardware Platforms 6 Neural Networks and Data Sets 8 CPU Scalability: FCN Synthetic CPU Scalability: FCN Real CPU Scalability: CNN Synthetic CPU Scalability: CNN Real CPU Scalability: RNN LSTM GPU Scalability: FCN Synthetic GPU Scalability: FCN Real 14 GPU Scalability: CNN Synthetic GPU Scalability: CNN Real 16 GPU Scalability: RNN LSTM

Hardware Platforms



- Use one quad-core desktop CPU (i.e., Intel i7-3820 CPU @ 3.60GHz) and two 8-core server-grade CPUs (i.e., Intel Xeon CPU E5-2630 v3 @ 2.40GHz)
- Use two generations of GPU cards, GTX 1080 @ 1607MHz with Pascal architecture, and Telsa K80 @ 562MHz with Kepler architecture

Computational Unit	Cores	Memory	OS	CUDA
Intel CPU i7-3820	4	64 GB	Ubuntu 14.04	-
Intel CPU E5-2630x2	16	128 GB	CentOS 7.2	-
GTX 980	2048	4 GB	Ubuntu 14.04	8.0
GTX 1080	2560	8 GB	Ubuntu 14.04	8.0
Telsa K80 GK210	2496	12 GB	CentOS 7.2	8.0

Figure: The experimental hardware settings for numerical tests

Neural Networks and Data Sets



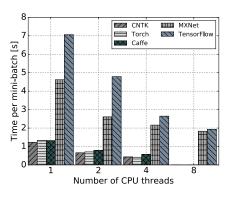
- A large fully-connected neural network (FCN-S) with around 55 million parameters is used to evaluate the performance of FCN
- The classical AlexNet (AlexNet-S) is used as an representative of CNN
- A smaller FCN (FCN-R) is constructed for MNIST data set
- An AlexNet (AlexNet-R) architecture is used for Cifar10 data set
- For RNNs, considering that the main computation complexity is related to the length of input sequence, 2 LSTM layers are selected for testing, with input length of 32.

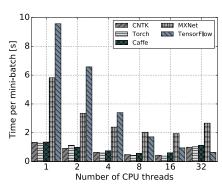
Networks		Input	Output	Layers	Parameters	
FCN	FCN-S	26752	26752	5	~55 millions	
FCN	FCN-R	784	10	5	~31 millions	
CNN	AlexNet-S	150528	1000	4	~61 millions	
CNN	AlexNet-R	3072	10	4	~81 thousands	
RNN	LSTM	10000	10000	2	~13 millions	

Figure: The experimental setup of neural networks for synthetic data and real data

CPU Scalability: FCN Synthetic







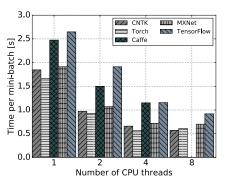
(a) Results on i7-3820.

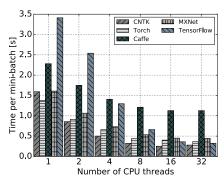
(b) Results on E5-2630.

Figure: FCN-S performance comparison on CPU platform with a mini-batch size of 64 (The lower the better)

CPU Scalability: FCN Real







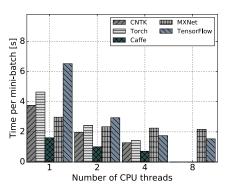
(a) Results on i7-3820.

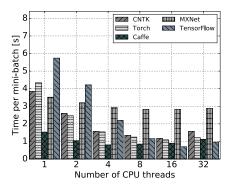
(b) Results on E5-2630.

Figure: The FCN-R performance comparison on CPU platform with a mini-batch size of 1024 (The lower the better)

CPU Scalability: CNN Synthetic







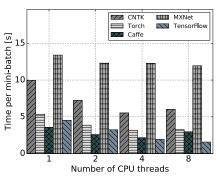
(a) Results on i7-3820.

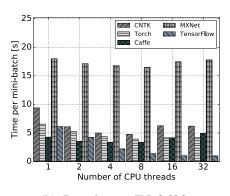
(b) Results on E5-2630.

Figure: AlexNet-S performance comparison on CPU platform with a mini-batch size of 16 (The lower the better)

CPU Scalability: CNN Real







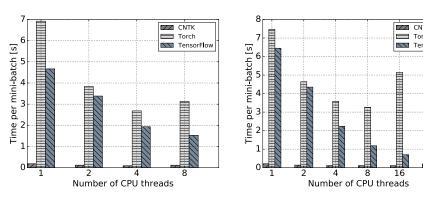
(a) Results on i7-3820.

(b) Results on E5-2630.

Figure: AlexNet-R performance comparison on CPU platform with a mini-batch size of 1024 (The lower the better)

CPU Scalability: RNN LSTM





(a) Results on i7-3820.

(b) Results on E5-2630.

Figure: LSTM performance comparison on CPU platform with a mini-batch size of 256 (The lower the better)

GPU Scalability: FCN Synthetic



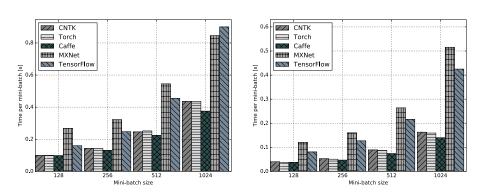


Figure: The performance comparison of FCN-S on GPU platforms

GPU Scalability: FCN Real



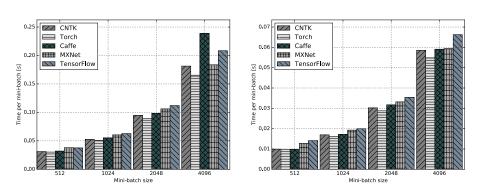


Figure: The performance comparison of FCN-R on GPU platforms

GPU Scalability: CNN Synthetic



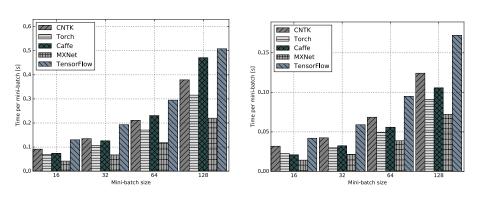


Figure: The performance comparison of AlexNet-S on GPU platforms

GPU Scalability: CNN Real



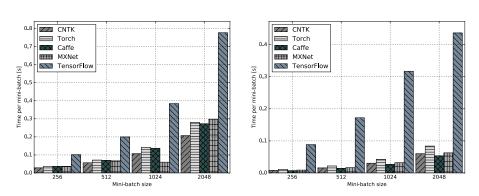


Figure: The performance comparison of AlexNet-R on GPU platforms

GPU Scalability: RNN LSTM



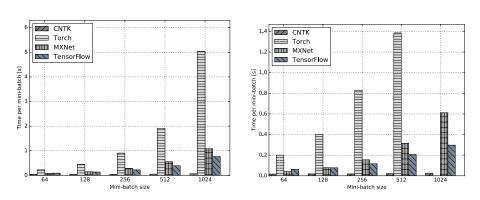


Figure: The performance comparison of LSTM on GPU platforms

§3. Python

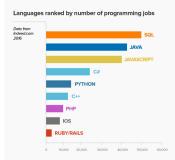
- 18 Python: A general-purpose programming language
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- 21 Control Flow
- 22 Modules
- 23 Additional Comments



Python: A general-purpose programming language



- Created by Guido van Rossum in 1989 and first released in 1991
- Named after "the Monty Python" (British comedy group)
- An interpreted language—simple, clear, and readable
- Python has many excellent packages for machine learning
- The language of choice in introductory programming courses



Feb	Change \$	Programming language	\$	Share \$	Trends \$
1		Java		22.6 %	-1.3 %
2		Python		14.7 %	+2.8 %
3		PHP		9.4 %	-1.2 %
4		C#		8.3 %	-0.3 %
5	↑ ↑	Javascript		7.7 %	+0.4 %
6		С		7.0 %	-0.2 %
7	↓↓	C++		6.9 %	-0.6 %
8		Objective-C		4.2 %	-0.6 %
9	1	R		3.4 %	+0.4 %
10	1	Swift		2.9 %	+0.1 %

Python for Scientific Computing



Why Python for scientific computing?

- Dynamic data types and automatic memory management
- Full modularity, supporting hierarchical packages
- Strong introspection capabilities¹
- Exception-based error handling

Why consider such a slow language for simulation?

- Good for proof-of-concept prototyping
- Implementation time versus execution time
- Code readability and maintenance short code, fewer bugs
- Well-written Python code is "fast enough" for most computational tasks
- Time critical parts executed through compiled language or available packages

¹Code introspection is the ability to examine classes, functions and keywords to know what they are, what they do and what they know. Python provides several functions and utilities for code introspection, like dir(), help(), type().

Built-in Data Structures



Numeric types: int, float, complex

```
1 b=1L # long int
2 c=0xf # int (hex format)
3 d=010 # int (octal format)
4 e=1.0 # float
5 f=1+2j # complex
```

Sequence types: list, tuple, str, dict

```
t = (3.14, True, 'Yes', [1], (0xf,)) # tuple example
t = [3.14, True, 'Yes', [1], (1L, 0xf)] + [None]*3 # list example
s = "Hello' + ", " + 'world!' # str example 1
s = ("Hello, " "world!") # str example 2
d = [1: 'int', 'pi': 3.14] # dict example
s = "Python"; s.find('thon') # find substring
```

Formatted output

```
print('%(lang)s has %(num)02d quote types.' %{"lang":"Python", "num":3})
```

User defined functions²³

```
1 def square(x):
return x*x
```

²Function overhead is high. Not to call a function repeatedly; Using aggregation instead.

³Python always passes (the value of) the reference to the object to the function.

Control Flow



If-then-else

For loop

```
1  # loop from 0 to 9
2  for i in range(10):
        print i
4  
5  # loop over the list named by oldlist
6  newlist = [s.upper() for s in oldlist]
```

While loop

Modules



This way will only introduce the name 'math' into the name space in which the
import command was issued. The names within the math module will not
appear in the enclosing namespace: they must be accessed through the name
math.

```
import math math. sin (3.14)
```

• This way does not introduce the name math into the current namespace. It does introduce all public names of the math module into the current namespace.

```
from math import * sin(3.14)
```

• This will only import the sin function from math module and introduce the name sin into the current namespace, but it will not introduce the name math into the current namespace, directly use

```
from math import sin sin (3.14)
```

 Make it as local as possible to avoid import overhead; But avoid calling it repeatedly; If possible, avoid it!

Additional Comments



• In Python, everything (including functions, modules, and files) are objects. A variable is created through assignment:

```
x = y = z = 0.1
```

help() is a function which gives information about the object. For example,

```
help('modules') # generate a list of all modules that can be imported help('modules time') # generate a list of modules with 'time' in description
```

Use a profiler to find optimization possibilities

```
import profile  # cProfile is now recommended
profile.run('main()')
```

- Some useful and important packages
 - NumPy: for scientific computing
 - Matplotlib/Pylab: for visualising data
 - SciPy: providing lots of numerical algorithms
 - SymPy: for symbolic mathematics

§4. TensorFlow

- 24 Programming Interface
- 25 Computational Graph
- 26 Visualization: TensorBoard
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- 28 Example: SoftMax in TF (Cont)



Programming Interface



- Graph: In TensorFlow, machine learning algorithms are represented as computational graph. A computational or data flow graph is a form of directed graph where vertices or nodes describe operations, while edges represent data flowing between these operations.
- Operation: An operation may represent a mathematical equation, a variable or constant, a control flow directive, a file I/O operation or even a network communication port.
- Tensor: A tensor is a multi-dimensional collection of homogeneous values with a fixed, static type.
- Variable: Variables can be described as persistent, mutable handles to in-memory buffers storing tensors.
- Session: In TensorFlow the execution of operations and evaluation of tensors may only be preformed in a special environment called session.

Computational Graph



```
import tensorflow as tf
3
    graph = tf.Graph()
 4
 5
    with graph. as default():
6
         # Define two constants
7
         a = tf.constant(1.0)
8
         b = tf.constant(2.0)
9
10
         # Define an operation node: c = a * b
11
         c = tf.multiply(a, b)
12
         # Add scalar summary to operation node
13
         tf.summary.scalar('c', c)
14
15
         # Merge all the summaries and write to ./board
16
         merged = tf.summary.merge_all()
17
         writer = tf.summary.FileWriter('./board', graph)
18
19
     with tf. Session (graph=graph):
20
         # Write data to / board
21
         writer.add summary(merged.eval())
```

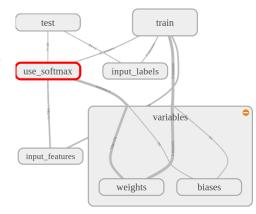


Visualization: TensorBoard



Computation graphs are powerful but complicated

- thousands of nodes or more
- network is deep
- graph visualization tool TensorBoard is helpful



Example: SoftMax in TF

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```
import tensorflow as tf
# Import training and test data
import tensorflow.examples.tutorials.mnist.input_data as input_data
mnist = input data.read data sets("MNIST data/", one hot=True)
# Create a new TensorFlow graph
graph = tf.Graph()
with graph.as default():
    # Nodes or entire subgraphs can be grouped into one visual block for tensorboard
    with tf.name_scope('input_features'):
        # Placeholder for input variables (None = variable dimension)
        x = tf.placeholder(tf.float32, shape=[None, 784], name='input x')
    with tf.name scope('input labels'):
        # Placeholder for labels
        y_ = tf.placeholder(tf.float32, shape=[None, 10], name='labels')
    with tf.name scope('variables'):
       W = tf. Variable(tf.zeros([784, 10]), name='weights')
        # Track tensor distributions over time for tensorboard
        tf.summary.histogram('WEIGHTS', W)
        b = tf. Variable(tf.zeros([10]), name='biases')
        tf.summary.histogram('BIASES', b)
    with tf.name scope('use softmax'):
        # Apply softmax regression model to the input data and get prediction v
        y = tf.nn.softmax(tf.matmul(x, W) + b)
```

Example: SoftMax in TF (Cont)

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```
with tf.name scope('train'):
       # Compute the cross entropy of real label y and prediction labe y
        cross entropy = -tf.reduce.sum(y *tf.log(y))
       # Create a gradient—descent optimizer with learning rate = 0.01
        train step = tf.train.GradientDescentOptimizer(0.01), minimize(cross entropy)
    with tf.name scope('test'):
        correct\_prediction = tf.equal(tf.argmax(y,1), tf.argmax(y_1))
        accuracy = tf.reduce mean(tf.cast(correct prediction, "float"))
        # Track tensor values over time for tensorboard
        tf.summary.scalar('Accuracy', accuracy)
   # Merge all the summaries and write to ./board
   merged = tf.summarv.merge all()
    writer = tf.summary.FileWriter('./board', graph)
with tf. Session (graph=graph) as sess:
   # Initialize all variables
    tf.global variables initializer().run()
    for step in range (1000):
        if (step \%10) == 0:
           # Feed test data to compute accuarcy
            feed = {x: mnist.test.images, v: mnist.test.labels}
           _, acc = sess.run([merged, accuracy], feed_dict=feed)
            print ('Accuracy at %s step: %s' %(step, acc))
        else.
           # Feed training data to train the model
            batch x, batch y = mnist.train.next batch (100)
            sess.run(train step, feed dict={x: batch x, y : batch y})
            writer.add_summary(merged.eval(feed_dict={x:batch_x, y_:batch}),
                               global step=step)
```

§5. MXNet

29 Programming Interface

30 Example: SoftMax in MXNet



31 Example: SoftMax in MXNet (Cont)

Programming Interface



- Support many scope applications (e.g. computer vision, natural language processing, speech recognition, unsupervised machine learning, support embedded APIs, visualization)
- Mixed programming style: imperative and declarative
 - Data parallelism with multi-devices: Better scalability than TensorFlow, reportedly
 - Support many different front-end, including JavaScript (so it be run on web browsers as well)
 - Provide intermediate-level and high-level interface modules
 - Provide abundant IO functions
- Second Fully compatible with Torch: modules and operators
- Support building neural network graphs
 - Call mx.viz.plot_network()
- Not well documented

Example: SoftMax in MXNet



```
import mxnet
    import mxnet.symbol as sym
    import numpy as np
    import numpy.random as random
    import time
    from minpy core import function
    from minpy core import grad and loss
8
    # define softmax symbol
    x shape = (num samples, num classes)
10
11
    label shape = (num samplesm.)
    softmax_symbol = sym. SoftmaxOutput(data=sym. Variable('x'),
12
                                        name='softmax', grad scale = 1.0/num samples)
13
14
15
    # convert MXNet symbol into a callable function
    # corresponding gradient function
16
    softmax = function(softmax_symbol, [('x', x_shape), ('softmax_label', label_shape)])
17
18
19
    # make softmax label;
    # MXNet's softmax operator does not use one-of-many label format
20
21
    softmax label = np.argmax(label, axis=1)
22
23
    # Redefine loss function using softmax as one operator
24
    def train loss (w. x):
25
        y = np.dot(x, w)
26
         prob = softmax(x=y, softmax label=softmax label)
27
         loss = -np.sum(label * np.log(prob)) / num samples
28
         return loss
```





```
# Initialize weight matrix (again)
weight = random.randn(num_features, num_classes)

# Calculate gradient function automatically
grad_function = grad_and_loss(train_loss)

# Now training it for 100 iterations
start_time = time.time()
for i in range(100):
    dw, loss = grad_function(weight, data)
    if i % 10 == 0:
        print 'Iter {}, training loss {}'.format(i, loss)
        weight == 0.1 * dw

print 'Training time: {}s'.format(time.time() - start_time)
```

§6. Torch

- 32 Programming Interface
- 33 Example: Two-Layer Network
- 34 Example: Two-Layer Network (Cont)
- 35 Example: Linear Regression in Lua
- 36 Example: Linear Regression in Lua (Cont)
- 37 Example: Linear Regression in Lua (Cont)



Programming Interface



- Wide range of applications
 - Speech, image and video applications
 - Large-scale machine-learning applications
- Fastest scripting language Lua is used
- Portable to any platform
 - Torch can run on iPhone with no modification to scripts
 - Embeddable, with ports to iOS, Android and FPGA backends
- Easy extensibility
 - Easy to integrate any library into Torch

Example: Two-Layer Network

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```
import torch
    from torch.autograd import Variable
    # N is batch size: D in is input dimension:
    # H is hidden dimension: D out is output dimension.
    N, D in, H, D out = 64, 1000, 100, 10
    # Create random Tensors to hold inputs and outputs, and wrap them in Variables.
9
    x = Variable(torch.randn(N, D in))
    y = Variable (torch.randn(N, D out), requires grad=False)
12
    # Use the nn package to define our model as a sequence of layers.
    model = torch.nn.Sequential(torch.nn.Linear(Din, H),
                                  torch.nn.ReLU().
                                  torch.nn.Linear(H. D out) )
    # The nn package also contains definitions of popular loss functions:
    loss fn = torch.nn.MSELoss(size average=False)
    learning rate = 1e-4
    for t in range (500):
        # Forward pass: compute predicted y by passing x to the model.
        v \text{ pred} = \text{model}(x)
        # Compute and print loss.
        loss = loss fn(y pred, y)
         print(t. loss.data[0])
        # Zero the gradients before running the backward pass
        model.zero grad()
```

Example: Two-Layer Network (Cont)



```
# Backward pass: compute gradient of the loss
loss.backward()

# Update the weights using gradient descent
for param in model.parameters():
    param.data = learning_rate * param.grad.data
end
end
```



Example: Linear Regression in Lua

```
require 'torch'
     require 'optim'
     require 'nn'
4
5
    # write the loss to a text file and read from there to plot it as training proceeds
    logger = optim.Logger('loss log.txt')
    # input data
    data = torch. Tensor \{\{40, 6, 4\}, \{44, 10, 4\}, \{46, 12, 5\},
    \{48, 14, 7\}, \{52, 16, 9\}, \{58, 18, 12\}, \{60, 22, 14\},
10
    {68, 24, 20}, {74, 26, 21}, {80, 32, 24}}
11
12
13
    # define the container
    model = nn. Sequential()
14
     ninputs = 2: noutputs = 1
15
16
17
    # define the only module
18
    model: add(nn. Linear(ninputs. noutputs))
19
20
    # Define a loss function
     criterion = nn. MSECriterion()
21
22
23
    # retrieve its trainable parameters
    x. dl dx = model: getParameters()
24
25
26
    # compute loss function and its gradient
27
     feval = function(x new)
28
       # set x to x_new, if differnt
29
        if x \sim = x new then
30
           x:copv(x new)
31
        end
```





```
32
        # select a new training sample
33
        nidx = (nidx or 0) + 1
34
        if nidx > (\#data)[1] then nidx = 1 end
35
36
        local sample = data[_nidx_]
37
        local target = sample[{ {1} }]
38
        local inputs = sample[{ {2.3} }]
39
40
        # reset gradients
41
        dl dx:zero()
42
43
        # evaluate the loss function and its derivative wrt x
44
        local loss x = criterion: forward (model: forward (inputs), target)
        model: backward(inputs, criterion: backward(model.output, target))
45
46
47
        # return loss(x) and dloss/dx
        return loss x . dl dx
48
49
    end
50
51
    # define SGD
52
    sgd_params = {
53
        learningRate = 1e-3,
54
        learningRateDecay = 1e-4,
55
        weightDecay = 0.
56
       momentum = 0
57
58
59
    # we cycle 10,000 times over our training data
     for i = 1.1e4 do
60
       #this variable is used to estimate the average loss
61
62
        current loss = 0
```



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```
#an epoch is a full loop over our training data
   for i = 1, (\#data)[1] do
      # return new x and value of the loss functions
      .fs = optim.sgd(feval.x.sgd params)
      # update loss
      current loss = current loss + fs[1]
   end
   # report average error on epoch
   current loss = current loss / (#data)[1]
   print('current loss = ' .. current loss)
   logger:add{['training error'] = current loss}
   logger: style {['training error'] = '-'}
   logger: plot()
end
# Test the trained model
text = \{40.32, 42.92, 45.33, 48.85, 52.37, 57, 61.82, 69.78, 72.19, 79.42\}
for i = 1.(\#data)[1] do
   local myPrediction = model: forward (data[i][{{2,3}}])
   print(string.format("%2d %6.2f %6.2f", i, myPrediction[1], text[i]))
end
```

§7. Caffe

38 Programming Interface

39 Example: Image Classification

40 Example: Extend Layers

41 Example: Extend Layers (Cont)

Caffe

Deep learning framework by BAIR

Programming Interface



- Mainly focus on (and well suited for) CNN and image recognition
- Expressive architecture
 - Define models and optimization by configuration without hard-coding
 - With protocol tool to define parameters for nets and solvers . . .
- Not well documented

Example: Image Classification



```
import caffe
    import matplotlib.pyplot as plt
3
4
    # paste vour image URL here
5
    my image url = "https://wikipedia/Orang Utan/2 C Malaysia. JPG"
6
    !wget -O image.jpg $my image url
7
    # transform it and copy it into the net
    image = caffe.io.load image('image.jpg')
10
    caffe.net.blobs['data'].data[...] = transformer.preprocess('data', image)
11
12
    # perform classification
13
    caffe . net . forward ()
14
    # obtain the output probabilities
15
16
    output prob = net.blobs['prob'].data[0]
17
18
    # sort top five predictions from softmax output
19
    top inds = output prob.argsort()[:: -1][:5]
20
21
22
     plt.imshow(image)
23
24
25
     print 'probabilities and labels:'
26
     zip(output prob[top inds], labels[top inds])
```

Example: Extend Layers

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```
import caffe
import numpy as np
class EuclideanLoss (caffe.layer):
    def setup(self, bottom, top):
        #check input pair
        if len(bottom) != 2:
            raise Exception ("Need two inputs to compute distance")
    def reshape (self, bottom, top):
        #check input dimensions match
        if bottom [0]. count != bottom [1]. count:
            raise Exception ("Inputs must have the same dimension")
        #difference in shape of inputs
        self.diff = np.zeros_like(bottom[0].data, dtype=np.float32)
        # loss output is scalar
        top[0].reshape(1)
    def forward (self, bottom, top):
        self.diff[...] = bottom[0].data - bottom[1].data
        top[0], data[...] = np.sum(self.diff**2)/bottom[0].num/2.
    def backward(self, top, propagate down, bottom):
        for i in range (2):
            if not propagate_down[i]:
                continue
            if i == 0
                sign = 1
            else:
                sign = -1
```

Example: Extend Layers (Cont)



```
31 bottom[i].diff[...] = sign.self.diff / bottom[1].num
```

Define a class in Python to extend Layer

