Software Packages for Deep Learning

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§1. Introduction

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Machine Learning



- 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
- Related fields: data mining, computational statistics, optimization, ...
- Fourth paradigm, big data, artificial intelligence, Internet of things, deep learning, ...

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 rather than discrete
- Density estimation
- Dimensionality reduction
- ...

Packages for General Machine Learning

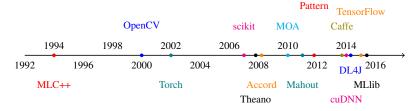


What is the purpose?

- 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: Pros and Cons



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

Popular Packages: Basic Information



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

- Other worth noting packages: CNTK/DMTK (Microsoft), PyTorch (beta)
- BVLC, Berkeley Vision and Learning Center
- DMLC, Distributed (Deep) Machine Learning Community, supported by Amazon, Intel, Microsoft, nVidia, Baidu, ...

Popular Packages: 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	Very few	
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	

§2. Numerical Comparisons

7 Hardware Platforms 8 Neural Networks and Data Sets 9 CPU Scalability: FCN Synthetic 10 CPU Scalability: FCN Real CPU Scalability: CNN Synthetic CPU Scalability: CNN Real **CPU Scalability: RNN** 13 GPU Scalability: FCN Synthetic 15 GPU Scalability: CNN Synthetic 16 GPU Scalability: CNN Real GPU Scalability: RNN Real 17

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 setting for data parallelization

Neural Networks and Data Sets



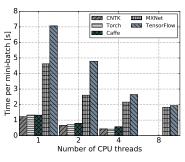
- A large fully-connected neural network (FCN-S) with around 55 million parameters is used to evaluate the performance of FCN
- The classical AlexNet (AlexNet-S) is used as an representative of CNN
- A smaller FCN (FCN-R) is constructed for MNIST data set
- An AlexNet (AlexNet-R) architecture is used 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.

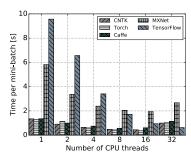
Networks		Input	Output	Layers	Parameters	
FC	FCN FCN-S		26752	26752	5	~55 millions
CN	N	AlexNet-S	150528	1000	4	~61 millions
FC	N	FCN-R	784	10	5	~31 millions
CN	N	AlexNet-R	3072	10	4	~81 thousands
RN	N	LSTM	10000	10000	2	~13 millions

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

CPU Scalability: FCN Synthetic





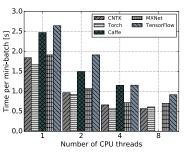


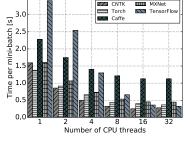
(a) Results on i7-3820.

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

CPU Scalability: FCN Real





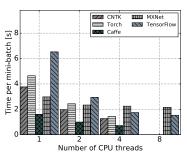


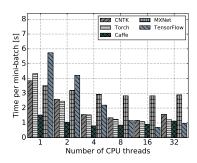
(a) Results on i7-3820.

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

CPU Scalability: CNN Synthetic





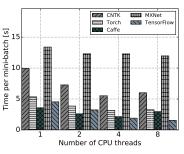


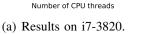
(a) Results on i7-3820.

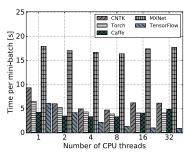
Figure: AlexNet-S performance comparison on CPU platform with a mini-batch size of 16 (The lower the better.)

CPU Scalability: CNN Real







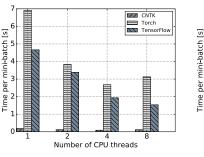


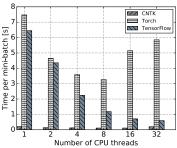
(b) Results on E5-2630.

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

CPU Scalability: RNN







(a) Results on i7-3820.

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

GPU Scalability: FCN Synthetic



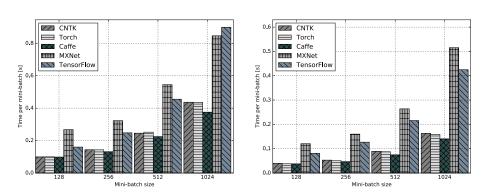


Figure: The performance comparison of FCN-S on GPU platforms.

GPU Scalability: CNN Synthetic



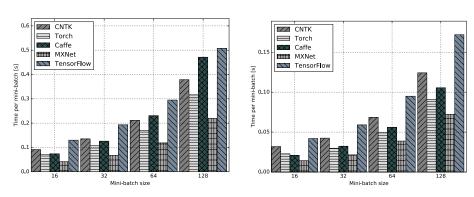


Figure: The performance comparison of AlexNet-S on GPU platforms.

GPU Scalability: CNN Real



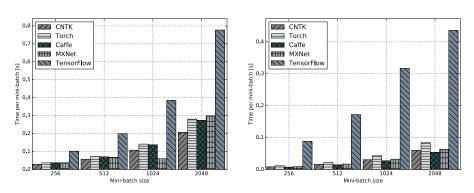


Figure: The performance comparison of AlexNet-R on GPU platforms.

GPU Scalability: RNN Real



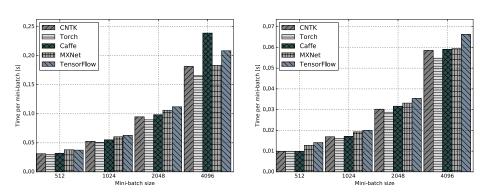


Figure: The performance comparison of FCN-R on GPU platforms.

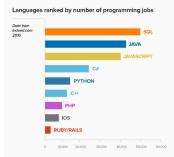
§3. Python

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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 2017	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		C		7.0 %	-0.2 %
7	$\downarrow \downarrow$	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().

Modules



Using 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. For example: math.sin(3.14).

```
1 import math
```

This way does not introduce the name math into the current namespace. It does however introduce all public names of the math module into the current namespace, directly using: sin(3.14)

```
1 from math import *
```

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 using: sin(3.14)

```
1 from math import sin
```

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

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

Formatted output

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

User defined functions

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

Control Flow



If-then-else

For loop

```
1 for i in range(10):
print i
```

While loop

Additional Comments



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

```
1 \quad x = y = z = 0.1
```

- When objects are passed to a function, Python always passes (the value of) the reference to the object to the function.
- help() is a function which gives information about the object. For example, help('modules') will generate a list of all modules which can be imported into the current interpreter.
- 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. Torch

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- 29 Example: Two-Layer Network
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Programming interface



- Wide range applications
 - Speech, image and video applications
 - Large-scale machine-learning applications
- Pastest scripting language Lua is used
- Easily ported to any platform
 - Torch can run on iPhone with no modification to scripts
- Easy extensibility
 - Easy to integrate any library into Torch



```
require 'torch'
    require 'optim'
    require 'nn'
5
    # write the loss to a text file and read from there
    # to plot the loss as training proceeds
    logger = optim.Logger('loss_log.txt')
8
9
    # input data
    data = torch. Tensor \{40, 6, 4\}, \{44, 10, 4\}, \{46, 12, 5\},
10
11
    \{48, 14, 7\}, \{52, 16, 9\}, \{58, 18, 12\}, \{60, 22, 14\},
    {68, 24, 20}, {74, 26, 21}, {80, 32, 24}}
12
13
14
    # define the container
15
    model = nn. Sequential()
    ninputs = 2; noutputs = 1
16
17
18
    # define the only module
    model: add(nn. Linear(ninputs, noutputs))
19
20
21
    # Define a loss function
22
     criterion = nn. MSECriterion()
```

23 24

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```
# retrieve its trainable parameters
x, dl_dx = model: getParameters()
# compute loss function and its gradient
feval = function(x new)
   # set x to x new, if differnt
   if x \sim = x new then
      x:copv(x new)
   end
# select a new training sample
   _{nidx_{-}} = (_{nidx_{-}} \text{ or } 0) + 1
   if nidx > (\#data)[1] then nidx = 1 end
   local sample = data[_nidx_]
   local target = sample[{ {1} }]
   local inputs = sample[{ {2,3} }]
# reset gradients
   dl dx:zero()
```



```
# evaluate the loss function and its derivative wrt x
43
        local loss x = criterion: forward (model: forward (inputs), target)
44
45
        model: backward (inputs, criterion: backward (model.output, target))
46
47
    # return loss(x) and dloss/dx
48
        return loss x, dl dx
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 1e4 times over our training data
60
    for i = 1.1e4 do
61
       #this variable is used to estimate the average loss
62
        current loss = 0
        #an epoch is a full loop over our training data
63
64
        for i = 1, (\#data)[1] do
65
           # return new x and value of the loss functions
           _, fs = optim.sgd(feval,x,sgd_params)
66
```



```
67
           # update loss
68
           current loss = current loss + fs[1]
69
        end
70
71
        # report average error on epoch
72
        current loss = current loss / (#data)[1]
73
        print('current loss = ' .. current loss)
74
75
        logger:add{['training error'] = current loss}
76
        logger: style {['training error'] = '-'}
77
        logger: plot()
78
    end
79
    # Test the trained model
80
    text = \{40.32, 42.92, 45.33, 48.85, 52.37, 57, 61.82, 69.78,
81
82
             72.19, 79.42}
83
84
    for i = 1, (\#data)[1] do
85
        local myPrediction = model: forward (data[i][{{2,3}}])
86
        print(string, format("%2d %6.2f %6.2f", i, myPrediction[1], text[i]))
87
    end
```

Example: Two-Layer Network



Example: Two-Layer Network

19

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```
learning rate = 1e-4
for t in range (500):
    # Forward pass: compute predicted y by passing x to the model.
    y \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()
         # 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
```

https://github.com/jcjohnson/pytorch-examples

§5. Caffe

31 Programming interface

32 Example: Image Classification

33 Example: Extend Layers

34 Example: Extend Layers

Programming interface



- Expressive architecture
 - Define models and optimization by configuration without hard-coding
 - With protocol tool to define parameters for nets and solvers . . .
- Support GPUs
- Mainly focus CNN for images
- Not well documented

Example: Image Classification



```
import caffe
    import matplotlib.pyplot as plt
3
 4
    # paste your image URL here
    my image url = "https://wikipedia/Orang Utan/2 C Malaysia. JPG"
    !wget -O image.ipg $mv 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
15
    # obtain the output probabilities
16
    output prob = net.blobs['prob'].data[0]
17
    # sort top five predictions from softmax output
18
    top inds = output prob.argsort()[:: -1][:5]
19
20
21
     plt.imshow(image)
22
     print 'probabilities and labels:'
23
    zip(output prob[top inds], labels[top inds])
```

Example: Extend Layers



```
import caffe
    import numpy as np
3
4
     class EuclideanLoss (caffe.layer):
5
         def setup(self, bottom, top):
6
             #check input pair
7
             if len(bottom) != 2:
8
                 raise Exception ("Need two inputs to compute distance")
9
10
         def reshape (self, bottom, top):
             #check input dimensions match
11
12
             if bottom [0]. count != bottom [1]. count:
13
                 raise Exception ("Inputs must have the same dimension")
             #difference in shape of inputs
14
15
             self.diff = np.zeros like(bottom[0].data, dtype=np.float32)
             # loss output is scalar
16
17
             top [0]. reshape (1)
18
19
         def forward (self, bottom, top):
20
             self.diff[...] = bottom[0].data - bottom[1].data
21
             top[0], data[...] = np.sum(self.diff**2)/bottom[0].num/2.
```

Example: Extend Layers



```
22
         def backward(self, top, propagate_down, bottom):
23
             for i in range (2):
24
                 if not propagate down[i]:
25
                      continue
                 if i == 0
26
27
                      sign = 1
28
                 else:
29
                      sign = -1
30
                 bottom[i].diff[...] = sign.self.diff / bottom[1].num
```

Define a class in Python to extend Layer

https://docs.google.com/presentation/d/1UeKXVgRvvxg9OUdh_UiC5G71UMscNPlvArsWER41PsU/edit#slide=id.gc2fcdcce7_216_0

§6. TensorFlow

- 35 Computational graph
- 36 Programming interface
- 37 Visualization: TensorBoard
- 38 Example 1: SoftMax
- 39 Example 1:SoftMax

Computational graph

11

12



```
import tensorflow as tf
    graph = tf.Graph()
    with graph. as default():
        a = tf.constant(1.0)
        tf.summary.scalar('aa', a)
        b = tf.constant(2.0)
        tf.summary.scalar('bb', b)
        c = tf.multiply(a, b)
        tf.summary.scalar('c', c)
13
        merged = tf.summary.merge_all()
         writer = tf.summary.FileWriter('./board', graph)
14
15
    with tf. Session (graph=graph):
16
         tf.global_variables_initializer().run()
17
18
         writer.add summary(merged.eval())
```



Figure: Computation graph

Programming interface



- Graph: In TensorFlow, machine learning algorithms are represented as computational graph. A computational or dataflow graph is a form of directed graph where vertices or nodes describe operations, while edges represent data flowing between these operations.
- Operation: An opreation 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.

Visualization: TensorBoard



Computation graphs are powerful but complicated

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

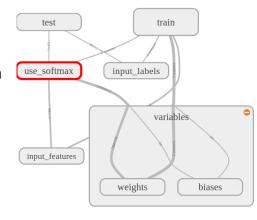


Figure: Graph Visualization



```
import tensorflow as tf
 2
3
    import tensorflow.examples.tutorials.mnist.input data as input data
4
    mnist = input data.read data sets("MNIST data/", one hot=True)
5
6
    graph = tf.Graph()
7
    with graph. as default():
         with tf.name scope('input features'):
9
             x = tf.placeholder(tf.float32, shape=[None, 784],
10
                                 name='input x')
11
12
         with tf.name_scope('input_labels'):
13
             y = tf.placeholder(tf.float32, shape=[None, 10],
14
                                 name='labels')
15
16
         with tf.name scope('variables'):
17
            W = tf. Variable(tf.zeros([784, 10]), name='weights')
             tf.summary.histogram('WEIGHTS', W)
18
             b = tf. Variable(tf.zeros([10]), name='biases')
19
20
             tf.summary.histogram('BIASES', b)
21
22
         with tf.name_scope('use_softmax'):
23
             y = tf.nn.softmax(tf.matmul(x, W) + b)
```



```
24
         with tf.name scope('train'):
25
             cross\_entropy = -tf.reduce\_sum(y\_*tf.log(y))
26
             train step = tf.train.GradientDescentOptimizer(0.01).minimize(cross entropy)
27
28
         with tf.name scope('test'):
29
             correct_prediction = tf.equal(tf.argmax(y,1), tf.argmax(y_1))
30
             accuracy = tf.reduce mean(tf.cast(correct prediction, "float"))
31
             tf.summary.scalar('Accuracy', accuracy)
32
        merged = tf.summary.merge_all()
33
         writer = tf.summary.FileWriter('./board', graph)
34
35
     with tf. Session (graph=graph) as sess:
36
         tf.global variables initializer().run()
37
         for step in range (1000):
38
             if (step \%10) == 0:
39
                 feed = {x: mnist.test.images, y: mnist.test.labels}
40
                 , acc = sess.run([merged, accuracy], feed dict=feed)
                 print ('Accuracy at %s step: %s' % (step. acc))
41
42
             else ·
43
                 batch x, batch y = mnist.train.next batch(100)
                 sess.run(train_step, feed_dict={x: batch_x, y_: batch_y})
44
45
                 writer.add summary(merged.eval(feed_dict={x: batch_x,
46
                                           y : batch y }), global step=step)
```

§7. MxNET

40 Programming interface

41 Example 1: SoftMax

Programming interface



- Mxnet.ndarray
 - Similar to numpy.ndarray
 - Supports both CPU and GPU
- Support building neural network graphs
 - Call mx.viz.plot_network()
- Mixed programing
 - Suport both imperative and declarative programming
- Provide intermediate-level and high-level interface modules
- Provide data parallelism with multi-devices
- Provide abundant IO functions
- Support many scope applications(e.g. computer vision, natural language processing, speech recognition, unsupervised machine learning, support embedded APIs, visualization)



```
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
9
10
    # define softmax symbol
    x shape = (num samples, num classes)
11
12
    label shape = (num samplesm.)
13
    softmax symbol = sym. SoftmaxOutput(data=sym. Variable('x'),
14
                        name='softmax', grad scale = 1.0/num samples)
15
16
    # convert MXNet symbol into a callable function
    # corresponding gradient function
17
    softmax = function(softmax symbol, [('x', x shape),
18
19
                      ('softmax label', label shape)])
20
21
    # make softmax label:
22
    # MXNet's softmax operator does not use one-of-many label format
23
    softmax label = np.argmax(label, axis=1)
```



```
# Redefine loss function using softmax as one operator
24
25
    def train loss (w, x):
        v = np.dot(x, w)
26
27
        prob = softmax(x=y, softmax_label=softmax_label)
28
         loss = -np.sum(label * np.log(prob)) / num samples
29
         return loss
30
31
    # Initialize weight matrix (again)
32
     weight = random.randn(num features, num classes)
33
34
    # Calculate gradient function automatically
35
     grad function = grad and loss(train loss)
36
37
    # Now training it for 100 iterations
38
     start time = time.time()
39
     for i in range (100):
        dw, loss = grad_function(weight, data)
40
41
        if i % 10 == 0:
42
             print 'Iter {}, training loss {}'.format(i, loss)
43
         weight -= 0.1 * dw
44
     print 'Training time: {}s', format(time, time() - start time)
```

