Software Packages for Deep Learning

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Outline

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
- ...

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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

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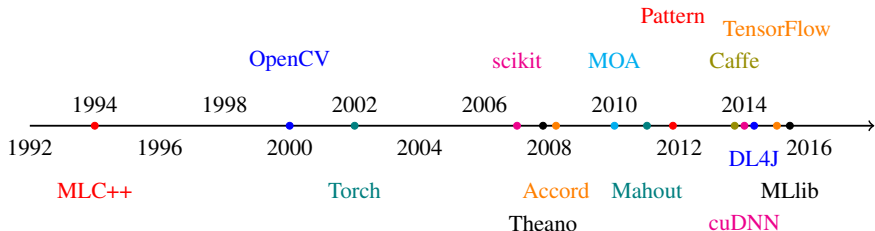
Deep Learning: Pros and Cons

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
- many hyper-parameters
- inefficient for categorical variables
- data hungry, learns slowly

Comparison: 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

- BVLC, Berkeley Vision and Learning Center
- DMLC, Distributed (Deep) Machine Learning Community, supported by Amazon, Intel, Microsoft, nVidia, Baidu, ...

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Comparison: Performance

NCMIS

| 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

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

Languages ranked by number of programming jobs

Data from Indeed.com 2016
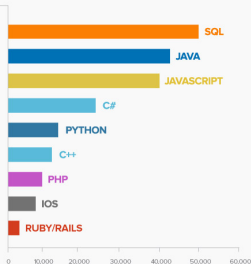
Feb 2017	Change	Programming language	Share	Trends
1		Java	22.6 %	-1.3 %
2		Python	14.7 %	+2.8 %
3		PHP	9.4 %	-1.2 %
4		C#	8.3 %	-0.3 %
5	↑↑	Javascript	7.7 %	+0.4 %
6		C	7.0 %	-0.2 %
7	↓↓	C++	6.9 %	-0.6 %
8		Objective-C	4.2 %	-0.6 %
9	↑	R	3.4 %	+0.4 %
10	↓	Swift	2.9 %	+0.1 %

Python for Scientific Computing

Why Python for scientific computing?

- Dynamic data types and automatic memory management
- Full modularity, supporting hierarchical packages
- Strong introspection capabilities[1]
- 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

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[1]Code 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().

Functions and Modules

Defining functions

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

Using modules

1. import math: This 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).

2. from math import *: This 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)

3. from math import sin: 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)

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], ())                   # 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

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

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Control Flow

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If-then-else

```
1  a = 1
2  if a > 0:
3      print "a is positive"
4  elif a=0:
5      print "a is zero"
6  else:
7      print "a is negative"
```

For loop

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

While loop

```
1  sum = 0; i = 0
2  while i < 10:
3      sum += i
4      i += 1
```

http://www.pythontutor.com

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Programming interface

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

Example 1:Linear-Regression

NCMIS

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

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Example 1:Linear-Regression

```
1  # retrieve its trainable parameters
2  x, dl_dx = model:getParameters()
3
4  # compute loss function and its gradient
5  feval = function(x_new)
6      # set x to x_new, if differnt
7      if x ~= x_new then
8          x:copy(x_new)
9      end
10
11  # select a new training sample
12      _nidx_ = (_nidx_ or 0) + 1
13      if _nidx_ > (#data)[1] then _nidx_ = 1 end
14
15      local sample = data[_nidx_]
16      local target = sample[{ {1} }]
17      local inputs = sample[{ {2,3} }]
18
19  # reset gradients
20      dl_dx:zero()
```

Example 1:Linear-Regression

```
1   # evaluate the loss function and its derivative wrt x
2       local loss_x = criterion:forward(model:forward(inputs), target)
3       model:backward(inputs, criterion:backward(model.output, target))
4
5   # return loss(x) and dloss/dx
6       return loss_x, dl_dx
7   end
8
9   # define SGD
10  sgd_params = {
11      learningRate = 1e-3,
12      learningRateDecay = 1e-4,
13      weightDecay = 0,
14      momentum = 0
15  }
16
17  # we cycle 1e4 times over our training data
18  for i = 1,1e4 do
19      #this variable is used to estimate the average loss
20      current_loss = 0
21      #an epoch is a full loop over our training data
22      for i = 1,(#data)[1] do
23          # return new x and value of the loss functions
24          _, fs = optim.sgd(feval, x, sgd_params)
```

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Example 1:Linear-Regression

```
 1          # update loss
 2          current_loss = current_loss + fs[1]
 3      end
 4
 5      # report average error on epoch
 6      current_loss = current_loss / (#data)[1]
 7      print('current loss = ' .. current_loss)
 8
 9      logger:add{['training error'] = current_loss}
10      logger:style{['training error'] = '-'}
11      logger:plot()
12  end
13
14  # Test the trained model
15  text = {40.32, 42.92, 45.33, 48.85, 52.37, 57, 61.82, 69.78,
16          72.19, 79.42}
17
18  for i = 1,(#data)[1] do
19      local myPrediction = model:forward(data[i][{{2,3}}])
20      print(string.format("%2d  %6.2f %6.2f", i, myPrediction[1], text[i]))
21  end
```

Programming interface

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

Example 1

Computational graph

TensorFlow computations are expressed as stateful dataflow graphs.

- each node corresponds to an operation (eg tensor, add, sub etc)
- each edge corresponds to tensor flowing direction

```
1   node1 = tf.constant(3.0, tf.float32)
2   node2 = tf.constant(4.0)
3   node3 = tf.add(node1, node2)
4   add_and_triple = adder_node * 3
```
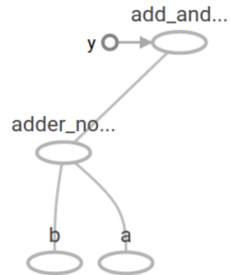

Figure: Computaion graph

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Programming interface

Visualization: TensorBoard

Computation graphs are powerful but complicated

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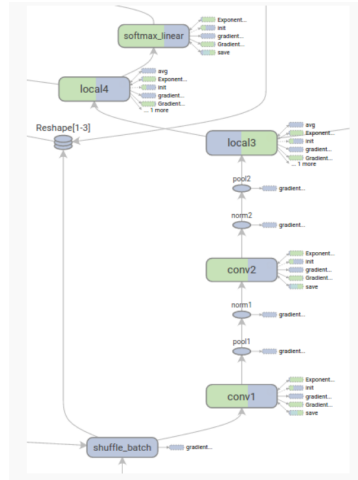- graph visualization tool TensorBoard is helpful

Figure: Graph Visualization

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Example 1: SoftMax

```
1   import tensorflow as tf
2
3   # Import the training data (MNIST)
4   import tf.examples.tutorials.mnist.input_data as input_data
5
6   # Possibly download and extract the MNIST data set
7   # Retrieve the labels as one-hot-encoded vectors
8   mnist = input_data.read_data_sets("MNIST_data/", one_hot=True)
9
10  # Create a new graph
11  graph = tf.Graph()
12
13  # Set our graph as the one to add nodes to
14  with graph.as_default():
15      # Placeholder for input variables (None = variable dimension)
16      x = tf.placeholder("float", shape=[None, 784])
17      # Placeholder for labels
18      y_ = tf.placeholder("float", shape=[None, 10])
19
20      # Weights and bias
21      W = tf.Variable(tf.zeros([784, 10]))
22      b = tf.Variable(tf.zeros([10]))
```

Example 1:SoftMax

```
1       # Apply softmax regression model
2       y = tf.nn.softmax(tf.matmul(x, W) + b)
3
4       # Compute the cross entropy of y_ and y
5       entropy = -tf.reduce_sum(y_*tf.log(y))
6       # Create a gradient-descent optimizer
7       train_step =
8           tf.train.GradientDescentOptimizer(0.01).minimize(entropy)
9
10      # Find the indices where the predictions were correct
11      correct_prediction = tf.equal(tf.argmax(y,1), tf.argmax(y_,1))
12      accuracy = tf.reduce_mean(tf.cast(correct_prediction, "float"))
13
14  with tf.Session(graph=graph) as session:
15      # Initialize all variables
16      tf.global_variables_initializer().run()
17
18      # Train the model
19      for step in range(1000):
20          batch_x, batch_y = mnist.train.next_batch(100)
21          train_step.run(feed_dict={x: batch_x, y_: batch_y})
22      # Print the accuracy using the model
23      print accuracy.run(feed_dict={x: mnist.test.images,
24                                    y_:mnist.test.labels})
```

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Programming interface

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

Example 1: SoftMax

```
1
2   import mxnet
3   import mxnet.symbol as sym
4   import numpy as np
5   import numpy.random as random
6   import time
7   from minpy.core import function
8   from minpy.core import grad_and_loss
9
10  # define softmax symbol
11  x_shape = (num_samples, num_classes)
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
17  # corresponding gradient function
18  softmax = function(softmax_symbol, [('x', x_shape),
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)
```

Example 1: SoftMax

```
1   # Redefine loss function using softmax as one operator
2   def train_loss(w, x):
3       y = np.dot(x, w)
4       prob = softmax(x=y, softmax_label=softmax_label)
5       loss = -np.sum(label * np.log(prob)) / num_samples
6       return loss
7
8   # Initialize weight matrix (again)
9   weight = random.randn(num_features, num_classes)
10
11  # Calculate gradient function automatically
12  grad_function = grad_and_loss(train_loss)
13
14  # Now training it for 100 iterations
15  start_time = time.time()
16  for i in range(100):
17      dw, loss = grad_function(weight, data)
18      if i % 10 == 0:
19          print 'Iter {}, training loss {}'.format(i, loss)
20      weight -= 0.1 * dw
21  print 'Training time: {}s'.format(time.time() - start_time)
```

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Numerical tests