A Simple Tutorial on Theano

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Outline

- What's Theano?
- How to use Theano?
  - Basic Usage: How to write a theano program
  - Advanced Usage: Manipulating symbolic expressions
- Case study 1: Logistic Regression
- Case study 2: Multi-layer Perceptron
- Case study 3: Recurrent Neural Network

WHAT'S THEANO?

Theano is many things

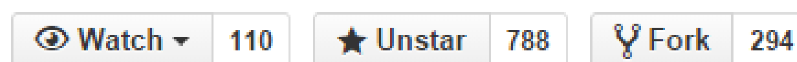
- Programming Language
- Linear Algebra Compiler
- Python library
  - Define, optimize, and evaluate mathematical expressions involving multi-dimensional arrays.

- Note: Theano is not a machine learning toolkit, but a mathematical toolkit that makes building downstream machine learning models easier.
  - Pylearn2

Theano features

- Tight integration with NumPy
- Transparent use of a GPU
- Efficient symbolic differentiation
- Speed and stability optimizations
- Dynamic C code generation

Project Status

- Theano has been developed and used since 2008, by LISA lab at the University of Montreal (leaded by Yoshua Bengio)
  - Citation: 202 (LTP: 88)
- Deep Learning Tutorials
- Machine learning library built upon Theano
  - Pylearn2
- Good user documentation
  - http://deeplearning.net/software/theano/
- Open-source on Github 

Basic Usage

HOW TO USE THEANO?

Python in 1 Slide

- Interpreted language
- OO and scripting language
- Emphasizes code readability
- Large and comprehensive standard library
- Indentation for block delimiters
- Dynamic type
- Dictionary
  - `d={‘key1’:‘val1’, ‘key2’:42, …}`
- List comprehension
  - `[i+3 for i in range(10)]`

NumPy in 1 Slide

- Basic scientific computing package in Python on the CPU
- A powerful N-dimensional array object
  - ndarray
- Sophisticated “broadcasting” functions
  - `rand(4,5) * rand(1,5) -> mat(4,5)`
  - `rand(4,5) * rand(4,1) -> mat(4,5)`
  - `rand(4,5) * rand(5) -> mat(4,5)`
- Linear algebra, Fourier transform and pseudorandom number generation

Overview of Theano

- Using Theano
  - Symbolically define mathematical functions
    - Automatically derive gradient expressions
  - Compile expressions into executable functions
    - theano.function([input params], output)
  - Execute expression

- Related libraries/toolkits:
  - Matlab, sympy, Mathematica

Installing Theano

- Requirements
  - OS: Linux, Mac OS X, Windows
  - Python: >= 2.6
  - Numpy, Scipy, BLAS
- pip install [--upgrade] theano
- easy_install [--upgrade] theano
- Install from source code
  - https://github.com/Theano/Theano

Building Symbolic Expressions

- Tensor
  - Scalars
  - Vectors
  - Matrices
  - Tensors
- Reductions
- Dimshuffle

Tensor

- Tensor: multi-dimensional array
  - Order of tensor: dimensionality
    - 0^{th}-order tensor = scalar
    - 1^{th}-order tensor = vector
    - 2^{th}-order tensor = matrix
    - …

Scalar math

```
from theano import tensor as T

# Note that theano is fully typed
x = T.scalar()
y = T.scalar()
z = x + y
w = z * x
a = T.sqrt(w)
b = T.exp(a)
c = a ** b
d = T.log(c)
```

Vector Math

```
from theano import tensor as T

x = T.vector()
y = T.vector()
# Scalar math applied elementwise
a = x * y
# vector dot product
b = T.dot(x, y)
```

Matrix Math

```
from theano import tensor as T

x = T.matrix()
y = T.matrix()
a = T.vector()
# Matrix-matrix product
b = T.dot(x, y)
# Matrix-vector product
c = T.dot(x, a)
```

Tensors

- Dimensionality defined by length of “broadcastable” argument
- Can add (or do other elemwise op) on two tensors with same dimensionality
- Duplicate tensors along broadcastable axes to make size match

```
from theano import tensor as T

tensor3 = T.Tensortype(broadcastable=(False,
False, False), dtype=‘float32’)
x = tensor3()
```

Reductions

```
from theano import tensor as T

tensor3 = T.Tensortype(broadcastable=(False, False,
False), dtype='float32')
x = tensor3()

total = x.sum()
marginals = x.sum(axis = (0, 2))
mx = x.max(axis = 1)
```

Dimshuffle

```
from theano import tensor as T

tensor3 = T.Tensortype(broadcastable=(False, False,
False), dtype=‘float32’)
x = tensor3()
y = x.dimshuffle((2,1,0))

a = T.matrix()
b = a.T
# same as b
c = a.dimshuffle((1,0))
# Adding to larger tensor
d = a.dimshuffle((0,1,’x’))
e = a + d
```

zeros_like and ones_like

- zeros_like(x) returns a symbolic tensor with the same shape and dtype as x, but with every element to 0

- ones_like(x) is the same thing, but with 1s

Compiling and running expressions

- theano.function
- shared variables and updates
- compilation modes
- compilation for GPU
- optimizations

theano.function

```
>>> from theano import tensor as T
>>> x = T.scalar()
>>> y = T.scalar()

>>> from theano import function
>>> # first arg is list of SYMBOLIC inputs
>>> # second arg is SYMBOLIC output
>>> f = function([x, y], x + y)

>>> # Call it with NUMERICAL values
>>> # Get a NUMERICAL output
>>> f(1., 2.)
array(3.0)
```

Shared variables

- A “shared variable” is a buffer that stores a numerical value for a theano variable
  - think as a global variable
- Modify outside function with get_value and set_value

Shared variable example

```
>>> from theano import shared
>>> x = shared(0.)
>>> from theano.compat.python2x import OrderedDict
>>> updates[x] = x + 1

>>> f = T.function([], updates=updates)

>>> f() # updates
>>> x.get_value()

>>> x.set_value(100.)
>>> f() # updates
>>> x.get_value()
```

Compilation modes

- Can compile in different modes to get different kinds of programs
- Can specify these modes very precisely with arguments to theano.function
- Can use a few quick presets with environment variable flags

Example preset compilation modes

- FAST_RUN
- FAST_COMPILE
- DEBUG_MODE

Optimizations

- Theano changes the symbolic expressions you write before converting them to C code
- It makes them faster
  - `(x+y) + (x+y) -> 2 * (x+y)`
- It makes them more stable
  - `exp(a) / exp(a).sum(axis=1) -> softmax(a)`

Optimizations

- Sometimes optimizations discard error checking and produce incorrect output rather than an exception

```
>>> x = T.scalar()
>>> f = function([x], x/x)
>>> f(0.)
array(1.0)
```

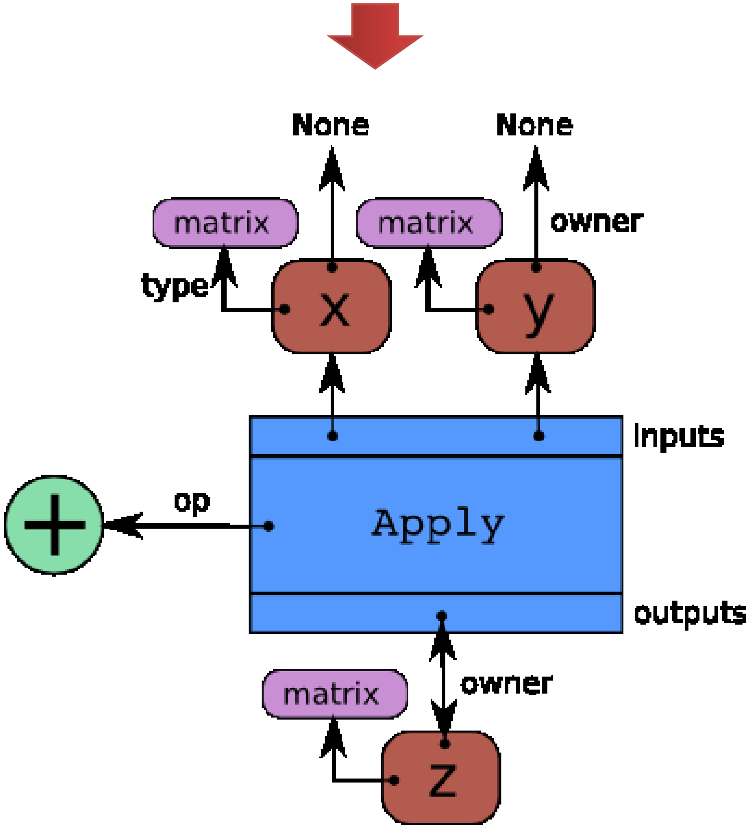
Advanced Usage

HOW TO USE THEANO?

Manipulating Symbolic Expressions

- Theano Graphs
  - variable nodes
  - op nodes
  - apply nodes
  - type nodes

```
x = T.dmatrix('x')
y = T.dmatrix('y')
z = x + y
```



Manipulating Symbolic Expressions

- Automatic differentiation
  - **`tensor.grad(func, [params])`**

```
>>> from theano import pp
>>> x = T.dscalar('x')
>>> y = x ** 2
>>> gy = T.grad(y, x)
>>> pp(gy)  # print out the gradient prior to optimization
'((fill((x ** 2), 1.0) * 2) * (x ** (2 - 1)))'
>>> f = function([x], gy)
>>> f(4)
array(8.0)
>>> f(94.2)
array(188.40000000000001)
```

The second argument of `grad()` can be a list (partial derivatives)

Loop: scan

- reduce and map are special cases of scan
  - scan a function along some input sequence, producing an output at each time-step.
  - Number of iterations is part of the symbolic graph
  - Slightly faster than using a *for* loop with a compiled Theano function

Loop: scan

- Example-1

```
import theano
import theano.tensor as T
import numpy as np

# define shared variables
k = theano.shared(0)
n_sym = T.iscalar("n_sym")

results, updates = theano.scan(lambda:{k:(k + 1)}, n_steps=n_sym)
accumulator = theano.function([n_sym], [], updates=updates, allow_input_downcast=True)

k.get_value()
accumulator(5)
k.get_value()
```

Loop: scan

- Example-2

```
import theano
import theano.tensor as T
import numpy as np

# defining the tensor variables
X = T.matrix("X")
W = T.matrix("W")
b_sym = T.vector("b_sym")

results, updates = theano.scan(lambda v: T.tanh(T.dot(v, W) + b_sym), sequences=X)
compute_elementwise = theano.function(inputs=[X, W, b_sym], outputs=[results])

# test values
x = np.eye(2, dtype=theano.config.floatX)
w = np.ones((2, 2), dtype=theano.config.floatX)
b = np.ones((2), dtype=theano.config.floatX)
b[1] = 2

print compute_elementwise(x, w, b)[0]

# comparison with numpy
print np.tanh(x.dot(w) + b)
```

Example-3

- computing the Jacobian matrix
  - Manually, we can use “scan”

```
>>> x = T.dvector('x')
>>> y = x ** 2
>>> J, updates = theano.scan(lambda i, y, x : T.grad(y[i], x), sequences=T.arange(y.shape[0]), non_sequences=[y,x])
>>> f = function([x], J, updates=updates)
>>> f([4, 4])
array([[ 8.,  0.],
       [ 0.,  8.]])
```

Example-4

- computing the Hessian matrix
  – Manually, we can use “scan”

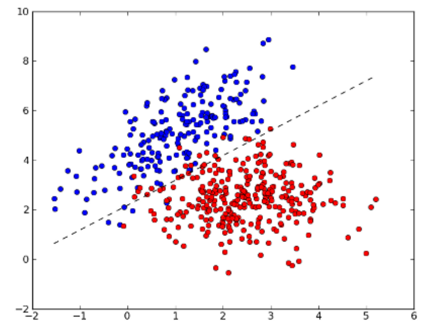
```
>>> x = T.dvector('x')
>>> y = x ** 2
>>> cost = y.sum()
>>> gy = T.grad(cost, x)
>>> H, updates = theano.scan(lambda i, gy,x : T.grad(gy[i], x),
sequences=T.arange(gy.shape[0]), non_sequences=[gy, x])
>>> f = function([x], H, updates=updates)
>>> f([4, 4])
array([[ 2.,  0.],
       [ 0.,  2.]])
```

Logistic Regression

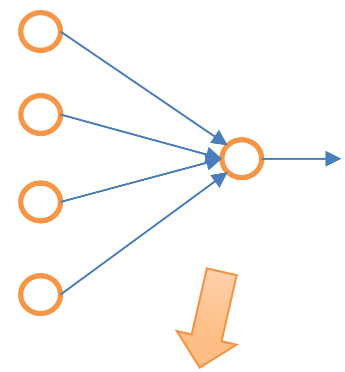
CASE STUDY - 1

Logistic Regression / Softmax

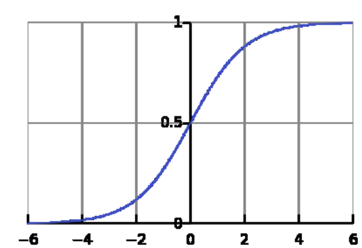
- Binary classification



- Discriminative function
  - $p(y=1|x) = \frac{1}{1+\exp(-w \cdot x - b)}$



- Objective function
  - Cross-entropy
    - $J = -y \cdot \log p - (1-y)\log(1-p)$



Logistic Regression

```
import numpy
import theano
import theano.tensor as T
rng = numpy.random

N = 400        # number of samples
feats = 784    # dimensionality of features
D = (rng.randn(N, feats), rng.randint(size=N, low=0, high=2))
```

x **y**

```
training_steps = 10000
```

Logistic Regression

```
# declare Theano symbolic variables
x = T.matrix(“x”)
y = T.vector(“y”)
w = theano.shared(rng.randn(784), name=“w”)
b = theano.shared(0., name=“b”)

print “Initial model:”
print w.get_value(), b.get_value()
```

Logistic Regression

```
# declare Theano symbolic variables
x = T.matrix(“x”)
y = T.vector(“y”)
w = theano.shared(rng.randn(100), name=“w”)
b = theano.shared(0., name=“b”)


# Construct Theano expression graph
p_1 = 1 / (1 + T.exp(-T.dot(x, w)-b)) # probability that target = 1
prediction = p_1 > 0.5                # the prediction threshold
xent = -y*T.log(p_1) – (1-y)*T.log(1–p_1) # cross-entropy loss func
cost = xent.mean() + 0.01 * (w**2).sum()  # the cost to minimize
gw, gb = T.grad(cost, [w, b])
```

Logistic Regression

```
x = T.matrix(“x”)
y = T.vector(“y”)
w = theano.shared(rng.randn(100), name=“w”)
b = theano.shared(0., name=“b”)
p_1 = 1 / (1 + T.exp(-T.dot(x, w)-b)
prediction = p_1 > 0.5
xent = -y*T.log(p_1) – (1-y)*T.log(1-p_1)
cost = xent.mean() + 0.01 * (w**2).sum()
gw, gb = T.grad(cost, [w, b])


# Compile
train = theano.function(
               inputs = [x, y],
               outputs = [prediction, xent]
               updates = {w : w-0.1*gw, b : b-0.1*gb})
predict = theano.function(inputs = [x], outputs = prediction)
```

Logistic Regression

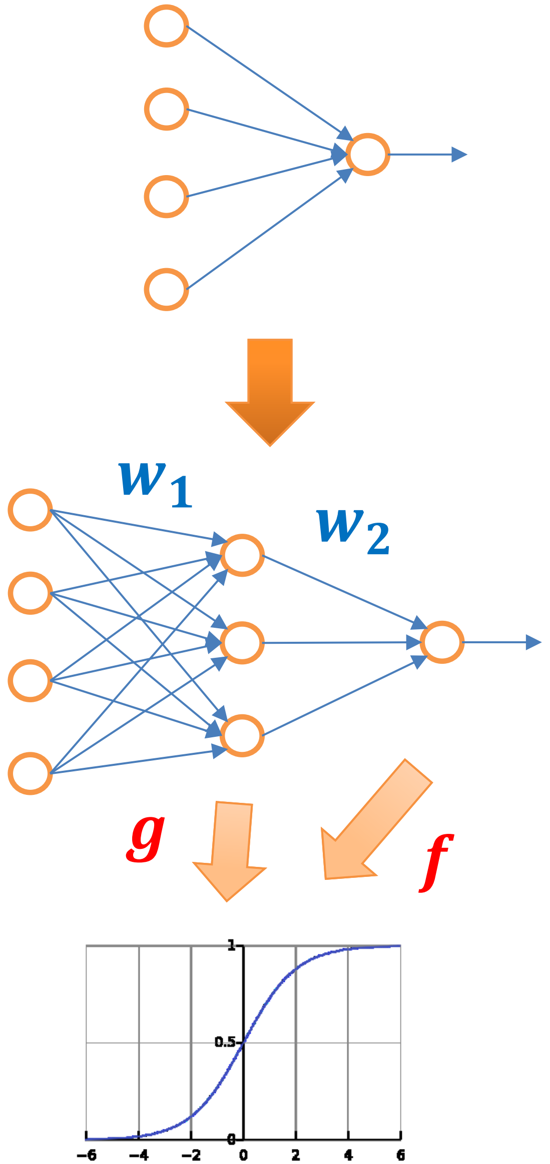
```
# Train
for i in range(training_steps):
      pred, err = train(D[0], D[1])

print “Final model:”
print w.get_value(), b.get_value()
print “target values for D: ”, D[1]
print “predictions on D: ”, predict(D[0])
```

Multi-Layer Perceptron

CASE STUDY - 2

Multi-Layer Perceptron

- Hidden layer(s)
- Discriminative function
  - $p(y=1|x) = \boldsymbol{f}(\boldsymbol{w_2} \cdot (\boldsymbol{g}(\boldsymbol{w_1} \cdot x + b_1) + b_2)$
  - $\boldsymbol{f}$ and $\boldsymbol{g}$ can be $sigmoid/tanh$ functions
- Objective function
  - Cross-entropy
    - $J = -y \cdot \log p - (1-y)\log(1-p)$



Multi-Layer Perceptron

```
import numpy
import theano
import theano.tensor as T
rng = numpy.random

N = 400       # number of samples
feats = 784   # dimensionality of features
D = (rng.randn(N, feats), rng.randint(size=N, low=0, high=2))
```

x **y**

```
training_steps = 10000
```

Multi-Layer Perceptron

```
# declare Theano symbolic variables
x = T.matrix(“x”)
y = T.vector(“y”)
w_1 = theano.shared(rng.randn(784,300), name=“w1”)
b_1 = theano.shared(numpy.zeros((300,)), name=“b1”)
w_2 = theano.shared(rng.randn(300), name=“w2”)
b_2 = theano.shared(0., name=“b2”)


print “Initial model:”
print w_1.get_value(), b_1.get_value()
print w_2.get_value(), b_2.get_value()
```

Multi-Layer Perceptron

```
# declare Theano symbolic variables
w_1 = theano.shared(rng.randn(784,300), name="w1")
b_1 = theano.shared(numpy.zeros((300,)), name="b1")
w_2 = theano.shared(rng.randn(300), name="w2")
b_2 = theano.shared(0., name="b2")


# Construct Theano expression graph
p_1 = T.sigmoid(-T.dot(T.sigmoid(-T.dot(x, w_1)-b_1), w_2)-b_2)
# probability that target = 1
prediction = p_1 > 0.5                # the prediction threshold
xent = -y*T.log(p_1) - (1-y)*T.log(1-p_1) # cross-entropy loss func
cost = xent.mean() + 0.01 * (w**2).sum()  # the cost to minimize
gw_1, gb_1, gw_2, gb_2 = T.grad(cost, [w_1, b_1, w_2, b_2])
```

Multi-Layer Perceptron

```
w_1 = theano.shared(rng.randn(784,300), name="w1")
b_1 = theano.shared(numpy.zeros((300,)), name="b1")
w_2 = theano.shared(rng.randn(300), name="w2")
b_2 = theano.shared(0., name="b2")
p_1 = T.sigmoid(T.dot(T.sigmoid(-T.dot(x, w_1)-b_1), w_2)-b_2)
prediction = p_1 > 0.5
xent = -y*T.log(p_1) – (1-y)*T.log(1–p_1)
cost = xent.mean() + 0.01 * (w**2).sum()
gw_1, gb_1, gw_2, gb_2 = T.grad(cost, [w_1, b_1, w_2, b_2])


# Compile
train = theano.function(
                 inputs = [x, y],
                 outputs = [prediction, xent]
                 updates = {w_1 : w_1-0.1*gw_1, b_1 : b_1-0.1*gb_1,
                            w_2 : w_2-0.1*gw_2, b_2 : b_2-0.1*gb_2})
predict = theano.function(inputs = [x], outputs = prediction)
```

Multi-Layer Perceptron

```
# Train
for i in range(training_steps):
      pred, err = train(D[0], D[1])

print “Final model:”
print w_1.get_value(), b_1.get_value()
print w_2.get_value(), b_2.get_value()
print “target values for D: ”, D[1]
print “predictions on D: ”, predict(D[0])
```

Recurrent Neural Network

CASE STUDY - 3

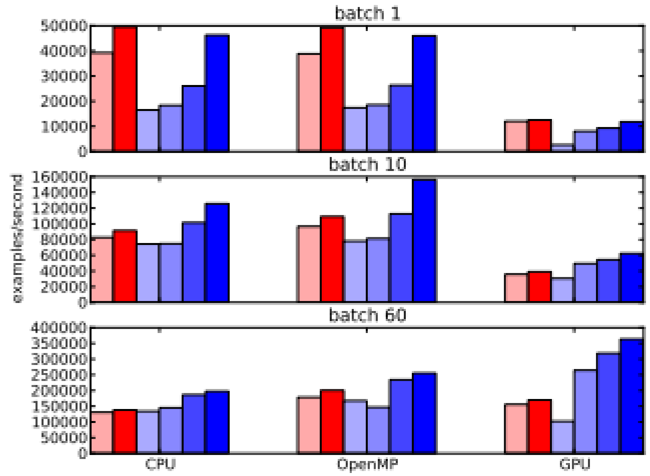
Recurrent Neural Network

- Exercise
  - Use $scan$ to implement the loop operation

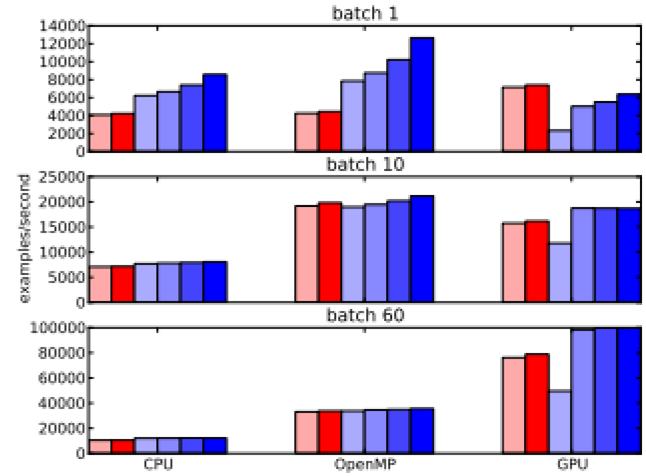
COMPARISON WITH OTHER TOOLKITS

Theano vs. Torch7

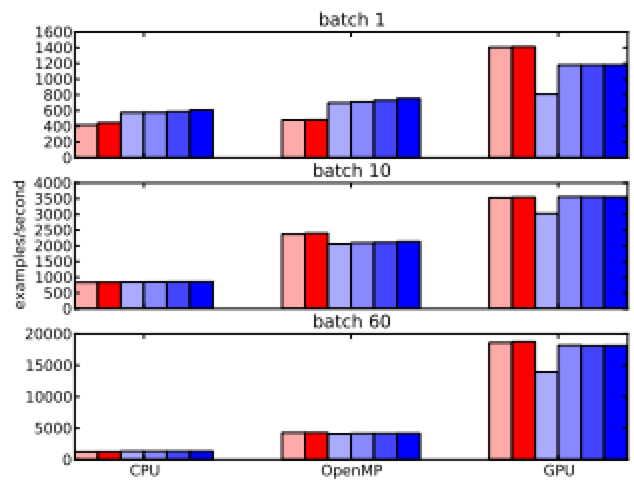
Features	Lua/Torch7	Python/Theano
Scripting language	✔	✔
Fast execution speed	✔	✔
Optimized BLAS, LAPACK	✔	✔
Plotting Environment	✔	✔ via matplotlib
GPU	✔ float only	✔ float only
Easy call to C functions	✔ Natively with Lua	✔ via Cython[a], `ctypes`, etc.
OS	Linux, MacOS X, FreeBSD	Linux, MacOS X, Windows
Public development	✔ on GitHub[b]	✔ on GitHub[c]
Unit tests	✔	✔ Buildbot[d], Travis-CI[e]
Used in published research	✔	✔
Used at companies	NEC	Google, Yahoo!, Card.io, startups
Sparse matrices	✘	✔
Symbolic differentiation	Non-symbolic NN gradient	✔
Differentiation over loop	✘	✔ Scan
R-operator	✘	✔ For most operations
Automatic graph optimization	✘	✔
Parallel functions	✔ OpenMP widely used	Only in BLAS and Conv2D
Embeddable in a C app.	✔	✘
Informative error messages	✔	Not always



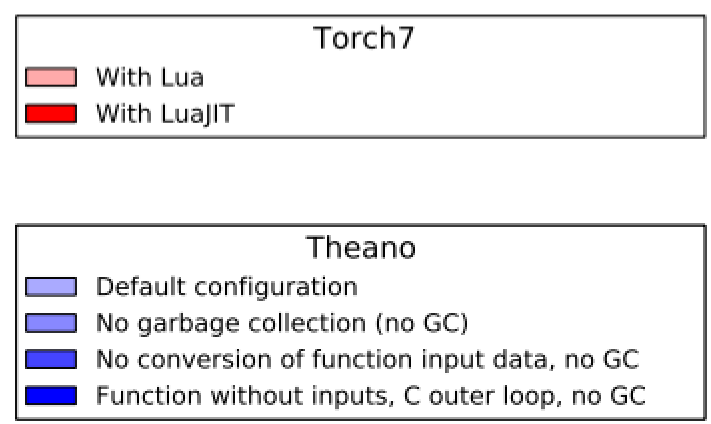
(a) Logistic regression



(b) Neural network, 1 hidden layer with 500 units



(c) Deep neural network, 3 hidden layers with 1000 units each



Thank you!