Instructor-Led Lab: Image Classification using the Theano Python Library

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GTC 2017



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Slides

github repo of this presentation https://github.com/nouiz/gtc2017/

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Modifying expressions

GPU

Debugging

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Convolution

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Exercise

Enc

High level

Python <- {NumPy/SciPy/libgpuarray} <- Theano <- {...}

- Python: OO coding language
- Numpy: n-dimensional array object and scientific computing toolbox
- SciPy: sparse matrix objects and more scientific computing functionality
- libgpuarray: GPU n-dimensional array object in C for CUDA and OpenCL(not ready!)
- ► Theano: compiler/symbolic graph manipulation
 - (Not a machine learning framework/software)
- ▶ {...}: Many libraries built on top of Theano

What Theano provides

- Lazy evaluation for performance
- GPU support
- Symbolic differentiation
- Automatic speed and stability optimization

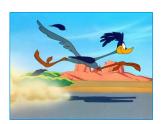
High level

Many [machine learning] library build on top of Theano

- Keras
- lasagne
- ► PyMC 3
- blocks
- sklearn-theano
- ▶ theano-rnn
- ► Morb

Goal of the stack

Fast to develop Fast to run



Some models build with Theano

Some models that have been build with Theano.

- Neural Networks
- Convolutional NN: CNN, AlexNet, OverFeat, GoogLeNet, Inception, ...
- Recurrent NN: RNN, CTC, LSTM, GRU, attention mechanisms, ...
- NADE, RNADE, MADE
- Autoencoders: AE, VAE, ...
- Generative Adversarial Nets
- SVMs
- many variations of above models and more

Project status

- ► Mature: Theano has been developed and used since January 2008 (9 yrs old)
- Driven hundreds of research papers
- Good user documentation
- Active mailing list with worldwide participants
- Core technology for Silicon-Valley start-ups
- Many contributors (some from outside our institute)
- Used to teach many university classes
- Used for research at big compagnies
- ▶ Theano 0.9 released 20th of March, 2017

Theano: deeplearning.net/software/theano/
Deep Learning Tutorials: deeplearning.net/tutorial/

Theano community

Active community

- Many people reply on our mailing lists
- Hundreds of answered questions on StackOverflow
- ▶ 123 contributors to Theano 0.9
- Main developers at MILA

Python

- General-purpose high-level OO interpreted language
- Emphasizes code readability
- Comprehensive standard library
- Dynamic type and memory management
- Easily extensible with C
- Slow execution
- Popular in web development and scientific communities

NumPy/SciPy

- ▶ NumPy provides an *n*-dimensional numeric array in Python
 - Perfect for high-performance computing
 - Slices of arrays are views (no copying)
- NumPy provides
 - Elementwise computations
 - Linear algebra, Fourier transforms
 - Pseudorandom number generators (many distributions)
- SciPy provides lots more, including
 - Sparse matrices
 - More linear algebra
 - Solvers and optimization algorithms
 - Matlab-compatible I/O
 - ▶ I/O and signal processing for images and audio

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Description

High-level domain-specific language for numeric computation.

- Syntax as close to NumPy as possible
- Compiles most common expressions to C for CPU and/or GPU
- Limited expressivity means more opportunities for optimizations
 - Strongly typed -> compiles to C
 - Array oriented -> easy parallelism
 - Support for looping and branching in expressions
 - No subroutines -> global optimization
- Automatic speed and numerical stability optimizations

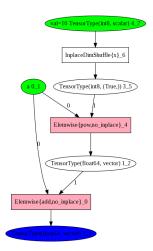
Description (2)

- Symbolic differentiation and R op (Hessian Free Optimization)
- Can reuse other technologies for best performance
 - CUDA, CuBLAS, CuDNN, BLAS, SciPy, PyCUDA, Cython, Numba, ...
- Works on Linux, OS X and Windows
- Multi-GPU (via platoon)
- New GPU back-end:
 - Float16 storage new back-end (need cuda 7.5)
 - Multi dtypes
 - Much simpler installation on Windows
- Extensive unit-testing and self-verification
- Extensible (You can create new operations as needed)

Simple example

```
import theano
# declare symbolic variable
a = theano.tensor.vector("a")
# build symbolic expression
b = a + a ** 10
# compile function
f = theano.function([a], b)
# Execute with numerical value
print f([0, 1, 2])
# prints 'array([0, 2, 1026])'
```

Simple example





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Overview of library

Theano is many things

- Language
- Compiler
- Python library

Scalar math

Some example of scalar operations:

```
import theano
from theano import tensor as T
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)
# Broadcasting (as NumPy, very powerful)
c = a + b
```

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

Using Theano:

- ▶ Dimensionality defined by length of "broadcastable" argument
- Can add (or do other elemwise op) 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 = T.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))
x = tensor3()
y = x.dimshuffle((2, 1, 0))
a = T. matrix()
b = a.T
# Same as b
c = a.dimshuffle((0, 1))
# Adding to larger tensor
```

d = a.dimshuffle((0, 1, 'x'))

Indexing

As NumPy! This mean slices and index selection return view

```
# return views, supported on GPU
a tensor[int]
a tensor[int, int]
a tensor[start:stop:step, start:stop:step]
a tensor[::-1] # reverse the first dimension
# Advanced indexing, return copy
a tensor[an index vector] # Supported on GPU
a tensor[an index vector, an index vector]
a tensor[int, an index vector]
a tensor[an index tensor, ...]
```

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Compiling and running expression

- ▶ theano function
- shared variables and updates
- compilation modes

theano.function

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

- It's hard to do much with purely functional programming
- "shared variables" add just a little bit of imperative programming
- ► A "shared variable" is a buffer that stores a numerical value for a Theano variable
- ► Can write to as many shared variables as you want, once each, at the end of the function
- Can modify value outside of Theano function with get_value() and set_value() methods.

Shared variable example

```
>>> from theano import shared
>>> x = shared(0.)
>>> updates = [(x, x + 1)]
>>> f = function([], updates=updates)
>>> f()
>>> x.get value()
1.0
>>> x.set value(100.)
>>> f()
>>> x.get value()
101.0
```

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

Interresting compilation configuration

Some Theano flags:

- mode=FAST_RUN: default. Fastest execution, slowest compilation
- mode=FAST_COMPILE: Fastest compilation, slowest execution. No C code.
- mode=DEBUG_MODE: Adds lots of checks.
- optimizer=fast_compile: mode=FAST_COMPILE with C code.
- optimizer=stabilize: optimizer=fast_compile with stability optimization.

Theano flags

Can be set globally:

- ▶ In a configuration file /.theanorc
- ► THEANO_FLAGS=mode=FAST_COMPILE python script.py

Sometimes as parameter of functions:

theano.function(..., mode="FAST_COMPILE")

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Modifying expressions

There are "macro" that automatically build bigger graph for you.

- theano.grad
- Others

Those functions can get called many times, for example to get the 2nd derivative.

The grad method

```
>>> x = T. scalar('x')
>>> y = 2. * x
>>> g = T.grad(y, x)
# Print the not optimized graph
>>> theano.printing.pydotprint(g)
 val=2.0 TensorType(float32, scalar)
                            name=x TensorType(float64, scalar)
                 0 TensorType(float32, scalar) /1 TensorType(float64, scalar)
                      Elemwise{mul,no_inplace}
                                                val=1.0 TensorType(float64, scalar)
             1 TensorType(float32, scalar) 0 TensorType(float64, scalar)
                                                       1 TensorType(float64, scalar)
                        Elemwise{second,no inplace}
                            O TensorType(float64, scalar)
              Elemwise{ mul}
                   TensorType(float64, scalar)
```

The grad method

```
>>> x = T. scalar('x')
>>> y = 2. * x
>>> g = T.grad(y, x)
# Print the optimized graph
>>> f = theano.function([x], g)
>>> theano.printing.pydotprint(f)
 val=2.0 TensorType(float64, scalar)
           TensorType(float64, scalar)
       DeepCopyOp
           TensorType(float64, scalar)
```

Others

- R_op, L_op for Hessian Free Optimization
- hessian
- jacobian
- clone the graph with replacement
- you can navigate the graph if you need (go from the result of computation to its input, recursively)

Enabling GPU

- ▶ libgpuarray (new-backend) supports all dtype
 - including float16 for storage
- Theano's old GPU back-end removed from the master of Theano
- ► CUDA supports float64, but it is slow on gamer GPUs

CuDNN

- ▶ V5 and V5.1 are supported
- ▶ V6 compile
- ▶ It is enabled automatically if available
- ► Theano flag to get an error if can't be used: "dnn.enabled=True"
- ► Theano flag to disable it: "dnn.enabled=False"

GPU: Theano flags

Theano flags allow to configure Theano. Can be set via a configuration file or an environment variable.

To enable GPU:

- Set "device=cuda" (or a specific GPU, like "cuda0")
- Set "floatX=float32"
- Optional: warn_float64={'ignore', 'warn', 'raise', 'pdb'}
- Instead of Theano flags, user can call "theano.gpuarray.use('cuda0')"

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floatX

Allow to change the dtype between float32 and float64.

- ▶ T.fscalar, T.fvector, T.fmatrix are all 32 bit
- ► T.dscalar, T.dvector, T.dmatrix are all 64 bit
- ► T.scalar, T.vector, T.matrix resolve to floatX
- floatX is float64 by default, set it to float32 for GPU

Debugging

- ▶ DebugMode: a mode that tests many things done by Theano (very slow)
- NanGuardMode: a mode that help find the cause of nan in the graph
- Error message
- theano.printing.debugprint: print a textual representation of computation
- profiling: To help know where time is spend

Error message: code

```
import numpy as np
import theano
import theano.tensor as T
x = T.vector()
y = T.vector()
z = x + x
z = z + y
f = theano.function([x, y], z)
f(np.ones((2,)), np.ones((3,)))
```

Error message: 1st part

```
Traceback (most recent call last):
[...]
ValueError: Input dimension mis-match.
    (input[0]. shape[0] = 3, input[1]. shape[0] = 2)
Apply node that caused the error:
   Elemwise{add, no inplace}(<TensorType(float64, vector)>,
                            <TensorType(float64, vector)>,
                            <TensorType(float64, vector)>)
Inputs types: [TensorType(float64, vector),
               TensorType(float64, vector),
               TensorType(float64, vector)]
Inputs shapes: [(3,), (2,), (2,)]
Inputs strides: [(8,), (8,), (8,)]
Inputs values: [array([1., 1., 1.]),
                array([ 1., 1.]),
                array([ 1., 1.])]
Outputs clients: [['output']]
```

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Error message: 2st part

HINT: Re-running with most Theano optimization disabled could give you a back-traces when this node was created. This can be done with by setting the Theano flags "optimizer=fast_compile". If that does not work, Theano optimizations can be disabled with "optimizer=None".

HINT: Use the Theano flag "exception_verbosity=high" for a debugprint of this apply node.

Error message: traceback

```
Traceback (most recent call last):
    File "test.py", line 9, in <module>
        f(np.ones((2,)), np.ones((3,)))
    File "/u/bastienf/repos/theano/compile/function_module.py",
        line 589, in __call__
        self.fn.thunks[self.fn.position_of_error])
    File "/u/bastienf/repos/theano/compile/function_module.py",
        line 579, in __call__
        outputs = self.fn()
```

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Error message: optimizer=fast_compile

```
Backtrace when the node is created: File "test.py", line 7, in <module> z = z + y
```

debugprint

```
>>> from theano.printing import debugprint
>>> debugprint(a)
Elemwise{mul, no_inplace} [id A] ''
| TensorConstant{2.0} [id B]
| Elemwise{add, no_inplace} [id C] 'z'
| < TensorType(float64, scalar)> [id D]
| < TensorType(float64, scalar)> [id E]
```

```
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Inputs

```
# Load from disk and put in shared variable.
datasets = load data(dataset)
train set x, train set y = datasets[0]
valid set x, valid set y = datasets[1]
# allocate symbolic variables for the data
index = T. Iscalar() # index to a [mini] batch
# generate symbolic variables for input minibatch
x = T. matrix('x') \# data, 1 row per image
y = T.ivector('y') # labels
```

Model

```
n in = 28 * 28
n \text{ out} = 10
# weights
W = theano.shared(
         numpy.zeros((n in, n out),
                      dtype=theano.config.floatX))
# bias
b = theano.shared(
         numpy.zeros((n out,),
                      dtype=theano.config.floatX))
```

Computation

```
# the forward pass
p_y_given_x = T.nnet.softmax(T.dot(input, W) + b)
# cost we minimize: the negative log likelihood
I = T.log(p_y_given_x)
cost = -T.mean(I[T.arange(y.shape[0]), y])
# the error
y_pred = T.argmax(p_y_given_x, axis=1)
err = T.mean(T.neq(y_pred, y))
```

Gradient and updates

Training function

```
# compile a Theano function that train the model
train model = theano.function(
    inputs=[index], outputs=(cost, err),
    updates=updates.
    givens={
        x: train set x[index * batch size:
                       (index + 1) * batch size],
        y: train set y[index * batch size:
                        (index + 1) * batch size]
```

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Inputs

```
# Load from disk and put in shared variable.
datasets = load_data(dataset)
train_set_x, train_set_y = datasets[0]
valid_set_x, valid_set_y = datasets[1]

# allocate symbolic variables for the data
index = T.lscalar() # index to a [mini]batch
```

y = T.ivector('y') # labels
Reshape matrix of shape (batch_size, 28 * 28)
to a 4D tensor, compatible for convolution

x = T. matrix('x') # the data, 1 row per image

layer0_input = x.reshape((batch_size, 1, 28, 28) $_2$)/66

image shape=(batch size, 1, 28, 28)

one bias per output feature map

b = theano.shared(b values)

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b values = numpy.zeros((filter shape[0],),dtype=...

Computation

```
# convolve input feature maps with filters
conv out = nnet.conv2d(input=x, filters=W)
# pool each feature map individually,
# using maxpooling
pooled out = pool.pool 2d(
    input=conv out,
    ds=(2, 2), // poolsize
    ignore border=True)
output = T.tanh(pooled out +
                b. dimshuffle('x', 0, 'x', 'x'))
```

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What is Lasagne

Lasagne is a thin framework/library on top of Theano. http://lasagne.readthedocs.org/

- Does not hide Theano
- Easily build Theano graphs by using layers
- Contains many preimplemented losses and optimizers
- ► Does not include a training loop

Lasagne MLP Example: Input Variables

```
input_var = T.tensor4('inputs')
target_var = T.ivector('targets')
```

```
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Lasagne MLP Example: Model

```
# Input and dropout layer
net = lasagne.layers.lnputLayer(
    shape=(None, 1, 28, 28), input var=input var)
net = lasagne.layers.DropoutLayer(net, p=0.2)
# Hidden layers and dropout:
nonlin = lasagne.nonlinearities.rectify
for in range(2):
    net = lasagne.layers.DenseLayer(
        network, 800, nonlinearity=nonlin)
    net = lasagne.layers.dropout(network, p=0.5)
# Output laver:
softmax = lasagne.nonlinearities.softmax
net = lasagne.layers.DenseLayer(network, 10,
    nonlinearity=softmax)
                                                 58 / 66
```

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Lasagne MLP Example: Train Function

```
pred = lasagne.layers.get output(network)
cat cross ent = lasagne.objectives.
    categorical crossentropy
loss = cat cross ent(pred, target_var)
loss = loss.mean()
params = lasagne.layers.get all params(
    network, trainable=True)
updates = lasagne.updates.nesterov momentum (
    loss, params, learning rate = 0.01,
    momentum = 0.9)
train fn = theano.function([input var, target var],
```

loss, updates=updates9/66

Lasagne MLP Example: Test Function

```
test pred = lasagne.layers.get output(
    network, deterministic=True)
test loss = cat cross ent(test pred, target var)
test loss = test loss.mean()
test acc = T.mean(T.eq(T.argmax(test pred, axis=1))
                       target var),
                  dtype=theano.config.floatX)
val fn = theano.function([input var, target var],
                         [test loss, test acc])
```

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ipython notebook

- Introduction
- Exercises (Theano only exercises)
- ▶ lenet (small CNN model to quickly try it)
- Reuse VGG16 features

Connection instructions

- Navigate to nvlabs.qwiklab.com
- Login or create a new account
- ► Select the "Instructor-Led Hands-on Labs" class
- Find the lab called "Theano" and click Start
- ► After a short wait, lab instance connection information will be shown
- Please ask Lab Assistants for help!

Further hands-on training

Check out the Self-Paced labs at the conference:

- Deep Learning, CUDA, OpenACC, Tools and more!
- Just grab a seat and take any available lab
- Located in the lower-level outside of LL20C

You will also receive Credits to take additional labs at nvidia.qwiklab.com

▶ Log in using the same account you used in this lab

Where to learn more

- Deep Learning Tutorials with Theano: deeplearning.net/tutorial
- ▶ Theano tutorial: deeplearning.net/software/tutorial
- ► Theano website: deeplearning.net/software
- ► Lasagne documentation: http://lasagne.readthedocs.io/
- ► You can also see frameworks on top of Theano like Blocks, Keras, Lasagne, ...

Questions, acknowledgments

Questions? Acknowledgments

- ► All people working or having worked at the MILA institute
- ► All Theano users/contributors
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